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Electronic and Optical Response of Zirconium Diboride with Intrinsic and Extrinsic Defects

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door

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Abstract

Zirconium diboride (ZrB_2) is an ultra-high temperature ceramic that combines metallic and covalent bonding, high thermal conductivity, and strong chemical stability, making it a promising material for applications such as pellicles, high-temperature coatings, and optoelectronic devices. In this thesis, the structural, electronic, and optical properties of pristine and defected ZrB_2 were investigated using density functional theory (DFT).

Pristine ZrB_2 was first characterized, with results showing metallic conductivity dominated by zirconium d states, strong covalent Zr–B bonding, and a plasmon peak at $\sim$6.5 eV. Intrinsic defects were then examined: boron vacancies were found to be energetically more favorable ($E_f = 3.38$ eV) than zirconium vacancies ($E_f = 5.39$ eV), consistent with their bonding nature. Extrinsic species were also studied. Oxygen and hydrogen adsorption were energetically favorable ($E_f = -0.54$ and -0.43 eV), while nitrogen adsorption was unfavorable. Copper incorporation was found to be possible on zirconium sites ($E_f = -0.57$ eV) but unlikely on boron sites.

Optical calculations revealed that both pristine and defected ZrB_2 maintain high EUV transparency, with $\sim$99% transmittance for a 50 nm film. Defects introduced only moderate modifications to the dielectric response: oxygen adsorption caused the strongest effect, shifting the plasmon peak downward by 0.2–0.3 eV, whereas other defects produced minor changes.

These results confirm the robustness of ZrB_2 against common point defects and support its suitability for high-performance optical and structural applications. They also highlight the importance of defect engineering, especially oxygen control, for optimizing its use in practical environments.

POPULAIRWETENSCHAPPELIJKE SAMENVATTING

De ontwikkeling van steeds kleinere computerchips vraagt om nieuwe technieken en materialen. Een belangrijk onderdeel hiervan is de zogenaamde pellicle, een dun beschermend membraan dat gebruikt wordt bij het belichten van chips met lasers. Zo'n pellicle moet vrijwel volledig doorzichtig zijn voor dit soort licht, maar tegelijkertijd bestand tegen hoge temperaturen en een zware chemische omgeving.

In dit onderzoek is met behulp van computermodellen gekeken naar zirkoniumdiboride ZrB_2, een keramisch materiaal dat bekendstaat om zijn uitzonderlijke hittebestendigheid en stabiliteit. Met behulp van quantummechanische berekeningen is onderzocht hoe het materiaal zich gedraagt, zowel in perfecte vorm als wanneer er onzuiverheden of defecten aanwezig zijn. Zulke defecten kunnen bijvoorbeeld ontstaan door ontbrekende atomen of door kleine hoeveelheden zuurstof, waterstof of stikstof die zich aan het oppervlak binden.

De resultaten laten zien dat ZrB_2 in zijn zuivere vorm al zeer geschikt is voor toepassing als pellicle: het dunne beschermlaagje dat in de chipproductie wordt gebruikt om kwetsbare onderdelen te beschermen. Het materiaal laat bijna al het benodigde licht door. Ook met de meeste defecten blijft het stabiel en behoudt het goede optische eigenschappen. Vooral zuurstof bleek echter een sterke invloed te hebben, wat suggereert dat controle over zuurstofverontreiniging cruciaal is voor een betrouwbare werking.

Dit onderzoek bevestigt dat ZrB_2 een veelbelovende kandidaat is voor toekomstige toepassingen in de halfgeleiderindustrie, en laat zien hoe computermodellen kunnen helpen om de invloed van atomaire defecten te begrijpen en materialen doelgericht te verbeteren.

1 Introduction

The development of new materials is important for pushing forward from semiconductors and aerospace parts to medical tools and energy applications [1]. With high-performing materials, we can build faster microchips, stronger and lighter components, improved implants, and more advanced systems for storing and converting energy. In the past, finding these materials was mostly done through experiments, where scientists had to make and test each material over and over. It works, but it takes a lot of time and money. Nowadays, computational methods have changed the game by making it possible to predict out material properties even before making anything in the lab. One of the main tools for this is density functional theory (DFT), which is a quantum mechanical method to calculate material properties like electronic structures, total energy, and other related properties directly from theory [2]. DFT helps us understand how stable a material is, what its band structure looks like, how defects behave, and even how it might interact with light [3]. Using these kinds of simulations speeds up the search for useful materials.

1.1 Two-Dimensional Materials

One class of materials where computational modelling, and particularly density functional theory, has played a major role is in the prediction and design of novel two-dimensional (2D) materials. These materials, which consist of atomically thin layers, often show physical and chemical properties that differ strongly from their bulk counterparts. Their high surface-to-volume ratio, quantum confinement effects, and tunable electronic structures have enabled breakthroughs in flexible electronics, optoelectronics, catalysis, and energy storage technologies [4, 5, 6, 7]. The discovery of graphene inspired the search for other layered materials such as transition metal dichalcogenides (TMDs) and hexagonal boron nitride (h-BN), many of which have since been studied extensively using DFT before being realised experimentally.

Within this landscape, two-dimensional transition metal borides (also referred to as MBenes) have attracted attention as a class of 2D materials that combine desirable properties of both metals and ceramics [8]. Their layered structures consist of alternating planes of transition metals and boron atoms, bonded by strong covalent and metallic interactions. As a result, borides exhibit high hardness, excellent thermal and electrical conductivity, chemical stability, and resistance to oxidation [9, 10]. These features make them promising candidates for extreme-environment applications, including high-temperature coatings, thermal protection systems, and optoelectronic devices.

Zirconium diboride (ZrB_2) is one such material and can be considered in both bulk and reduced dimensional forms. Studying its structural, electronic, and optical properties, both pristine and with defects, can help determine its suitability for advanced applications such as pellicles and high-performance coatings.

1.2 Zirconium Diboride as a High-Performance Material

Zirconium diboride (ZrB_2) is a transition metal boride that mixes both metallic and ceramic features, which makes it a strong candidate for use in demanding environments [11, 10]. It is one of the most stable compounds in the Zr-B system, from convex hull simulations [12], and it forms a hexagonal AlB_2-type structure with lattice constants of $a = b = 3.1677$ Å and $c = 3.5294$ Å [12]. The structure itself is made up of repeating hexagonal layers of boron and planes of zirconium, which are held together by strong covalent and metallic bonding. Because of these strong Zr-B covalent bonds, ZrB_2 has a very high melting point at 3246 °C [13], and it also shows impressive hardness and resistance to oxidation [11]. On top of that, it has good thermal stability and high thermal conductivity [14], making it useful in systems that need efficient heat dissipation and mechanical strength at high temperatures. In terms of mechanics, ZrB_2 is part of the group known as ultra-high temperature ceramics, with a Young's modulus of around 498 GPa at room temperature [15].

Because of its unusual mix of thermal, mechanical, and chemical properties, plus decent optical characteristics, ZrB_2 has been considered as a possible material for pellicles [16, 17]. As can be seen in Figure 1, both zirconium and boron have low atomic absorption cross-sections for EUV light, which points to a certain level of transparency in that spectral region [18]. Beyond pellicles, 2D borides in general have been proposed for a variety of other applications where their high thermal

conductivity, mechanical strength, and chemical stability are advantageous. These include use in high-temperature structural components, wear-resistant coatings, thermal protection systems, and even in certain optoelectronic or energy storage devices [9, 10]. By considering multiple types of applications, the scope of this work extends beyond optical transparency, aiming to provide a broader understanding of the structural, electronic, and optical properties of ZrB_2 in both pristine and defected forms.

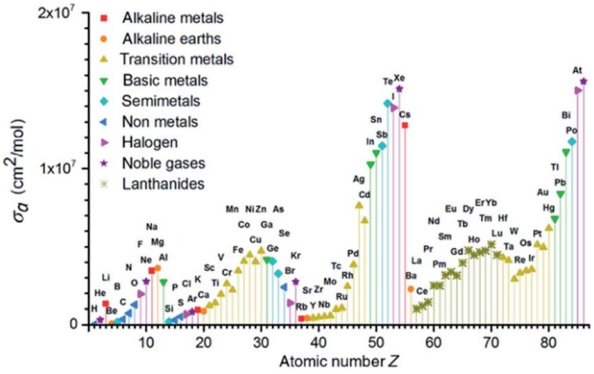


Figure 1: Atomic absorption cross-section of EUV light for elements with atomic numbers $Z = 1$ to 86. Figure reproduced from reference [18].

Still, in real-life situations, materials are hardly ever perfect. Most samples end up containing some kind of defect, either from how they were made or from being exposed to their environment [19]. These flaws can have a big impact on the structure, electronic properties, and even the optical behavior of ZrB_2, so it's important to take them into account when deciding if the material is suitable for high-performance uses.

Point defects, whether intrinsic or extrinsic, are a powerful way to tailor the properties of a material. Introducing dopants or vacancies can significantly modify a material's electronic structure, optical response, and thermodynamic stability [20]. For example, vacancies may change carrier concentrations or disrupt thermal transport, while dopants can introduce new energy states, alter absorption spectra, or improve chemical resistance. In the case of ZrB_2, tuning these properties is particularly relevant for its potential applications: optical transparency and stability are critical for pellicles, high hardness and oxidation resistance are essential for high-temperature coatings, and controlled electronic and optical behaviour is valuable for optoelectronic devices.

In this work, we examine three types of point defects in ZrB_2: vacancies and dopants. Vacancy defects occur when an atom is missing from its normal site in the lattice, and in this study we focus on both boron and zirconium vacancies. For dopants, we consider atoms like hydrogen, nitrogen, oxygen, and copper, which are placed in either interstitial or substitutional positions in the ZrB_2 structure. These cases give us a representative mix of intrinsic and extrinsic defects, allowing us to assess how different types and locations of defects affect the material's structural, electronic, and optical properties.

The goal of this thesis is to provide a comprehensive understanding of ZrB_2 in both pristine and defected forms. Using density functional theory, we study how the presence of vacancies and dopants changes its stability, electronic structure, and dielectric response. These results can guide future optimisation of ZrB_2 for advanced applications: for pellicles, the focus is on maintaining high optical transparency in the EUV range and mechanical stability under radiation; for high-temperature coatings, key requirements are thermal stability, oxidation resistance, and hardness; and for optoelectronic devices, tunable band structure and controlled dielectric properties are essential.

2 Computational methods

This section provides an overview of the numerical methods used to investigate the structural, electronic, and optical properties of ZrB_2 in both pristine and defected forms. Using density functional theory (DFT), we first assessed the stability of the bulk material, determined its structural parameters, and analysed its electronic structure. We then examined the formation energies of intrinsic defects

(vacancies) and extrinsic defects (dopants) to evaluate their stability. For each stable configuration, we calculated the corresponding electronic band structure and dielectric response to understand how these defects influence the material's overall performance. The main tools used for these calculations were GPAW [21] and ASE [22]. GPAW is a Python-based DFT package that uses the projector augmented wave (PAW) method, while ASE offers a flexible environment for setting up, running, and analyzing atomistic simulations.

2.1 Density Functional Theory

DFT is a commonly used quantum mechanical approach for computing the electronic structure of systems with many electrons. It makes it possible to calculate the electron density $\rho(\vec{r})$ from first principles, and from that, derive a variety of material properties such as total energy, band structure, and optical behavior [23].

The basic idea behind DFT comes from the two Hohenberg–Kohn theorems [24], which justify using the electron density as the main quantity in electronic structure calculations, instead of the full many-electron wavefunction. According to the first theorem, the external potential $V_{\text{ext}}(\vec{r})$ is uniquely determined by the ground-state electron density $\rho(\vec{r})$, except for a constant. This means that all ground-state properties are functionals of $\rho(\vec{r})$, and the problem becomes much simpler, reducing from $3N$ variables (for N electrons) to just three spatial ones.

The second theorem introduces a variational principle for the energy functional $E[\rho]$, which reaches its minimum at the true ground-state density. This is useful because it allows us to find the ground-state energy and density by minimizing the total energy:

$$E_0 = \min_{\rho \to N} \left(F[\rho] + \int \rho(\vec{r}) V_{\text{ext}}(\vec{r})\, d\vec{r} \right), \tag{1}$$

where $F[\rho]$ is a universal functional that contains the kinetic and electron-electron interaction energies.

These theorems are important because they turn the difficult many-electron Schrödinger equation into a more manageable minimization problem. This makes it possible to do accurate calculations for real materials without dealing with the full complexity of many-body wavefunctions.

Although the Hohenberg–Kohn theorems provide the theoretical basis, the method was made practical by Kohn and Sham [25], who introduced a way to solve the problem by replacing the interacting electron system with a system of non-interacting electrons that have the same ground-state density. The total energy functional in this case is written as:

$$F[\rho] = T_s[\rho] + J[\rho] + E_{\text{XC}}[\rho], \tag{2}$$

where $T_s[\rho]$ is the kinetic energy of the non-interacting system, $J[\rho]$ is the classical Coulomb energy, and $E_{\text{XC}}[\rho]$ is the exchange-correlation energy, which includes all the effects that come from many-body interactions not captured by the simpler terms.

From this, the Kohn–Sham equations are derived as:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + v_{\text{eff}}(\vec{r}) \right) \psi_i(\vec{r}) = \epsilon_i \psi_i(\vec{r}), \tag{3}$$

with the effective potential given by:

$$v_{\text{eff}}(\vec{r}) = v_{\text{ext}}(\vec{r}) + \int \frac{\rho(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|}\, d\vec{r}\,' + \frac{\delta E_{\text{XC}}[\rho]}{\delta \rho(\vec{r})}. \tag{4}$$

Then, the total electron density is obtained from the occupied Kohn–Sham orbitals:

$$\rho(\vec{r}) = \sum_i |\psi_i(\vec{r})|^2. \tag{5}$$

One of the main challenges in DFT is how to properly approximate the exchange-correlation functional $E_{\mathrm{XC}}[\rho]$. This term includes the complex quantum effects of electron exchange and correlation that go beyond the classical Coulomb interaction. Exchange comes from the Pauli exclusion principle, which makes electrons with the same spin avoid each other, and correlation describes how electrons move to avoid repulsion. Since the exact form of $E_{\mathrm{XC}}[\rho]$ is not known, we need to use approximations (see Section **??** for details on the functional tests carried out in this work). A common one is the local density approximation (LDA), which assumes that the exchange-correlation energy only depends on the local electron density. Another popular method is the generalized gradient approximation (GGA), which also takes into account the gradient of the density to capture non-uniform effects [26].

Each of these choices introduces certain errors. For instance, LDA often overbinds atoms and underestimates band gaps, while GGA tends to give better geometries and energies but still underestimates band gaps. Even with these limitations, DFT is still one of the most commonly used and effective methods in computational materials science. It provides a good balance between accuracy and efficiency for calculating the structural, electronic, and optical properties of materials.

2.2 Defect and Adsorption Energy

A key quantity for understanding how stable different point defects are is the defect formation energy. This value shows how much energy it takes to create a certain defect inside the material. Generally, defects that have lower formation energies are more likely to show up under equilibrium conditions [27]. The formation energy of a defect is given by [27]:

$$E_f = E_{\mathrm{defect}} - \sum_i n_i \mu_i - E_{\mathrm{pristine}}, \tag{6}$$

where E_f is the defect formation energy, E_{defect} is the total energy of the supercell with the defect, and E_{pristine} is the total energy of the clean, perfect supercell. The middle term, $\sum_i n_i \mu_i$, accounts for the atoms that are added or removed when making the defect. In this term, n_i tells how many atoms of element i were added ($n_i > 0$) or removed ($n_i < 0$), and μ_i is the chemical potential of that element in its standard state.

Since DFT simulations use periodic boundary conditions, defects in small supercells can interact with their own periodic images. This artificial interaction can influence the computed defect formation energy [27]. To reduce this problem, a convergence test was performed using progressively larger supercells until the defect formation energy was converged.

For extrinsic defects in the form of adsorbates—where atoms or molecules are bound to the surface or occupy interstitial sites—the stability is better described using the adsorption energy, E_{ads}. This is defined as:

$$E_{\mathrm{ads}} = E_{\mathrm{defect}} - E_{\mathrm{pristine}} - \sum_i n_i \mu_i, \tag{7}$$

where E_{defect} is the total energy of the system with the adsorbate, E_{pristine} is the total energy of the pristine host, and $\sum_i n_i \mu_i$ is the total energy of the isolated adsorbate atom or molecule. A negative adsorption energy indicates an energetically favourable adsorption process. This metric complements the defect formation energy analysis, providing insight into the stability of species that interact with the material surface.

2.3 Bader Charge Analysis

To evaluate the localization of defect-induced charge and to determine the minimum supercell size required for converged vacancy energetics, a Bader charge analysis was performed. The method partitions the total charge density into atomic volumes bounded by zero-flux surfaces in the gradient of the charge density [28]. This approach has become a standard way to quantify charge transfer in solids and

molecules, owing to its ability to provide chemically meaningful charges without relying on arbitrary basis functions [29, 30].

In this work, Bader charges were computed for pristine ZrB_2, as well as for supercells containing either a boron vacancy or a zirconium vacancy. The change in Bader charge relative to the pristine system was then analyzed for atoms in the first coordination shell and for atoms further away. This provided a measure of how localized the charge redistribution is around the defect, and whether defect images in smaller supercells interact with each other. In addition, charge-density difference maps were generated to visualize whether the missing or excess charge remained near the defect site or spread into the bulk of the material.

2.4 Dielectric Function

The dielectric function is a key property describing how a material responds to an external electromagnetic field. From it, several optical and electronic characteristics can be derived, including absorption, reflectivity, refractive index, and energy loss [23]. These quantities are important because they link directly to practical performance requirements: for pellicles, a high transmittance in the extreme ultraviolet (EUV) range is essential; for coatings, high reflectivity and stability under radiation are desirable; and for optoelectronic devices, the absorption profile determines possible operational wavelengths. In this work, the frequency-dependent complex dielectric function was determined to assess how point defects affect the optical response of ZrB_2 and, by extension, its suitability for these applications.

The dielectric function is defined per:

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega), \tag{8}$$

where $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ are the real and imaginary components. The real part shows the phase velocity of light inside the material, and the imaginary part is related to absorption [31].

The complex refractive index $n = \eta + i\kappa$ can be obtained from the dielectric function using $\epsilon(\omega) = n^2$, where η is the refractive index and κ the extinction coefficient:

$$\eta = \left\{ \frac{1}{2} \left[(\epsilon_1^2 + \epsilon_2^2)^{1/2} + \epsilon_1 \right] \right\}^{1/2}, \tag{9}$$

$$\kappa = \left\{ \frac{1}{2} \left[(\epsilon_1^2 + \epsilon_2^2)^{1/2} - \epsilon_1 \right] \right\}^{1/2}. \tag{10}$$

Then, the absorption coefficient α and the reflectivity R are computed as:

$$\alpha = \frac{2\omega\kappa}{c}, \qquad R = \frac{(1-\eta)^2 + \kappa^2}{(1+\eta)^2 + \kappa^2}, \tag{11}$$

where c is the speed of light in vacuum. Transmittance T for a thin film with thickness d can then be calculated as [31]:

$$T = \frac{(1-R)^2 e^{-\alpha d}}{1 - R^2 e^{-2\alpha d}}. \tag{12}$$

The dielectric function was calculated in GPAW [21] using the frequency-dependent linear response method. First, the ground-state was obtained by diagonalizing the Kohn–Sham Hamiltonian with a set number of bands. Based on convergence studies, 700 bands were used, as these yielded stable energy values, whereas higher bands showed abrupt energy jumps. The frequency grid was nonlinear, covering 10–20 eV with a step size of 0.02 eV. The plane-wave cutoff energy converged at 150 eV. Intraband effects were neglected because tests showed no significant impact on absorption. The broadening η was set to 0.05 eV after convergence testing. These parameters were applied consistently to both defective and pristine systems.

Electron Energy Loss Spectroscopy (EELS) provides complementary insight into the dielectric properties by revealing how much energy a fast electron loses when passing through the material,

mainly due to inelastic scattering [32, 33]. Peaks in the EELS spectrum correspond to characteristic excitation energies, such as plasmon resonances, interband transitions, and core-level excitations. In this context, EELS is particularly useful for identifying how defects in ZrB_2 shift or dampen these excitations, which in turn affects optical performance and electronic screening.

In theory, EELS is related to the dielectric function via the loss function:

$$L(\omega) = \mathrm{Im}\left[-\frac{1}{\epsilon(\omega)}\right], \tag{13}$$

which can also be written explicitly as:

$$L(\omega) = \frac{\epsilon_2(\omega)}{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)}. \tag{14}$$

Here, ϵ_1 and ϵ_2 are the real and imaginary parts of the dielectric function. In this study, the dielectric response for pristine and defected ZrB_2 was calculated as described above, and the EELS spectra were obtained via Equation 14. This analysis makes it possible to connect microscopic defect-induced changes in the dielectric function to experimentally measurable shifts in energy loss spectra.

3 Results

This section addresses the central research question introduced in the introduction: how stable is ZrB_2, and how do intrinsic and extrinsic point defects influence its structural, electronic, and optical properties? To answer this, we first establish reliable simulation parameters and characterise the pristine material as a baseline. The subsequent subsections then present the defect calculations, analysing how vacancies and dopants modify the stability, dielectric response, and electron energy loss spectrum of ZrB_2. First, the numerical settings and functional selection are validated, since these determine the reliability of the simulations. This includes convergence tests for plane-wave cutoff and k-point sampling, as well as an equation of state (EOS) fit to extract the bulk modulus and benchmark exchange–correlation functionals. These tests also serve to introduce important physical quantities, such as the bulk modulus, that are directly relevant for applications of ZrB_2. Next, the structural, electronic, and optical properties of pristine ZrB_2 are presented, providing a baseline for comparing the impact of defects. Finally, the formation energies, charge distribution, and electronic/optical properties of intrinsic point defects are analysed.

3.1 Convergence, Functional Selection, and Characterization of Pristine ZrB_2

In DFT simulations several settings must be checked before running large calculations to ensure that total energies and derived physical quantities are reliable. Higher numerical settings improve accuracy, but also increase computational cost, so convergence tests are essential.

Two of the most important parameters are the plane-wave energy cutoff and the k-point grid. To test the cutoff, a $2 \times 2 \times 2$ supercell of ZrB_2 was used. The total energy was calculated at different cutoffs. In Figure 2a, it can be seen that after 650 eV the change in energy is smaller than 1 meV.

Similarly, k-point sampling was tested by computing energies for increasing numbers of points in the Brillouin zone. The results (Figure 2b) show that a $5 \times 5 \times 5$ Monkhorst–Pack grid is sufficient for the $2 \times 2 \times 2$ cell. These settings were therefore chosen for all further simulations.

Another key property that can be used to benchmark computational parameters is the bulk modulus, which quantifies the resistance of a material to uniform compression. This parameter is especially relevant for ZrB_2 because of its proposed use in high-temperature structural and protective applications, where mechanical robustness is crucial.

The bulk modulus was extracted by fitting the energy–volume relation to the Birch–Murnaghan equation of state:

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 B_0' + \left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\}, \tag{15}$$

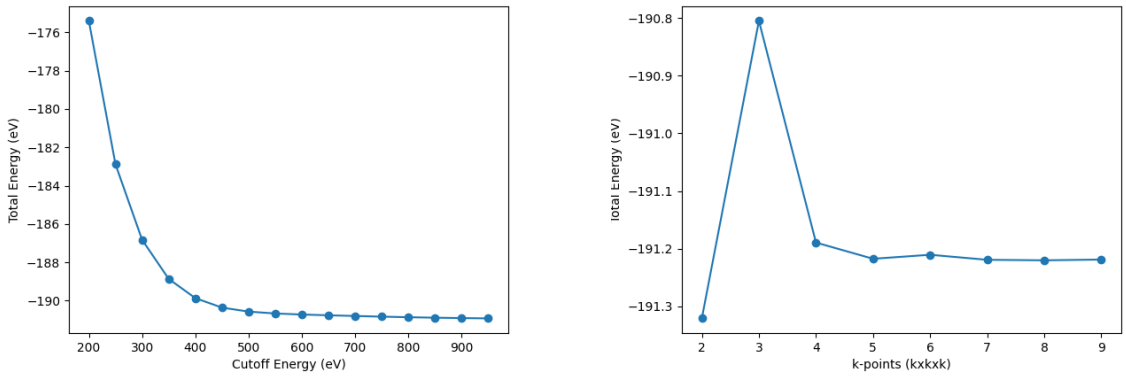


Figure 2: Convergence tests: (a) total energy vs. cutoff energy and (b) total energy vs. number of k-points for a $2 \times 2 \times 2$ supercell of ZrB_2.

where $E(V)$ is the total energy at volume V, E_0 is the equilibrium energy, V_0 is the equilibrium volume, B_0 is the bulk modulus at V_0, and $B_0^{'}$ is the pressure derivative of the bulk modulus.

Different exchange–correlation functionals were tested for ZrB_2, and the results are shown in Table 1. The Perdew–Burke–Ernzerhof (PBE) functional [26] gave a bulk modulus of 239.7 GPa, in excellent agreement with experimental data (∼240 GPa) [34]. Other functionals, such as RPBE and B3LYP, showed larger deviations. Based on this comparison, PBE was selected for all subsequent calculations in this project.

Table 1: Bulk modulus of ZrB_2 calculated using different exchange–correlation functionals, compared to experiment.

Functional	Bulk Modulus (GPa)
Experimental	240.1
PBE	239.7
RPBE	230.8
B3LYP	243.3

The optimized geometry of ZrB_2 forms a hexagonal AlB_2-type lattice with lattice parameters $a = b = 3.1677$ Å and $c = 3.5294$ Å, consistent with earlier studies [12]. The structure is made of layers of boron atoms in a hexagonal arrangement and zirconium atoms in between, figure 3. Strong covalent Zr–B bonds and metallic Zr–Zr interactions bind the layers together, giving rise to its ultra-high-temperature ceramic character [11]. The projected density of states (PDOS) in Figure 4 confirms

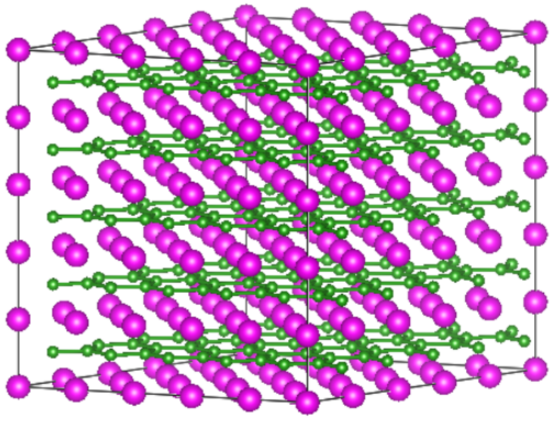


Figure 3: Structure of ZrB_2, where the pink atoms are Zr and the green atoms are B.

computationally that ZrB_2 behaves like a metal, with a non-zero density of states at the Fermi level. States near the Fermi energy are dominated by zirconium $3d$ orbitals, which provide the main metallic conductivity, while boron $2p$ orbitals lie further below the Fermi level and contribute primarily to bonding. Hybridization between Zr $3d$ and B $2p$ states below the Fermi level further confirms the mixed metallic–covalent bonding character of ZrB_2, consistent with previous computational and experimental reports on bulk and thin-film zirconium diboride [35, 10].

When compared to other two-dimensional transition-metal borides, metallic behavior is a common feature: TiB_2, HfB_2, and related diborides also show non-zero DOS at the Fermi level, with the transition-metal d orbitals playing the dominant role [10]. This trend suggests that metallic conductivity is intrinsic to the MBene family, arising from their layered structures and partially filled d states. For the applications considered here, metallicity is generally favorable: for pellicles it allows efficient dissipation of radiation-induced charges, for high-temperature coatings it contributes to thermal conductivity and mechanical robustness, and for optoelectronic contexts it ensures plasmonic and screening effects that can be tuned by defect engineering.

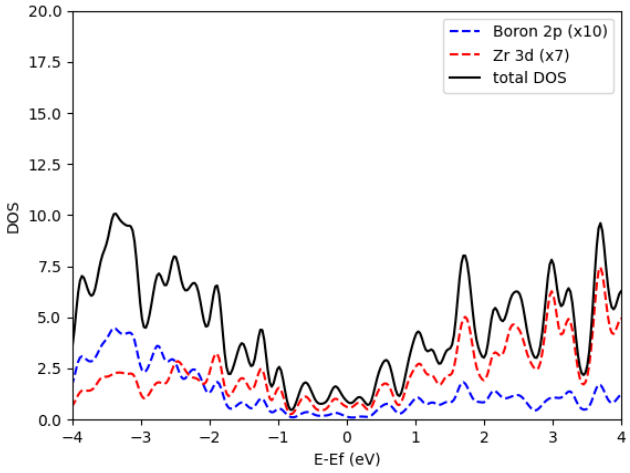


Figure 4: Projected density of states (PDOS) of pristine ZrB_2. The zirconium $3d$ states (red, scaled by 7) and boron $2p$ states (blue, scaled by 10) are shown alongside the total DOS (black).

3.2 Intrinsic Defects: Zirconium and Boron Vacancies

To assess the defect stability of ZrB_2, we first looked at intrinsic point defects in ZrB_2, namely zirconium and boron vacancies. These types of defects may form during synthesis, and in this section we evuluate whether they have a notable impact on the structural, electronic, or optical properties of the material.

An additional convergence test was carried out to figure out the smallest possible supercell size that avoids unwanted interactions between defect images. Since DFT simulations use periodic boundary conditions, small supercells can cause the defects to interact with their own periodic copies. To study this, vacancies were introduced in increasingly larger ZrB_2 supercells, and the formation energy was calculated for each one. Alongside this, a Bader charge analysis was done on every supercell to see how localized the defect-induced charge distribution is.

To investigate the link between cell size and defect energetics, Bader analysis was used. As shown in Figure 5, the formation energies for 3x3x4 to 4x4x5 supercells were lower compared to smaller ones. To try and explain this, a Bader charge analysis was again done , with the goal of checking if charge localization might play a role in these energy differences.

Figure 6 shows the minimum charge difference as a function of supercell size, for both boron and

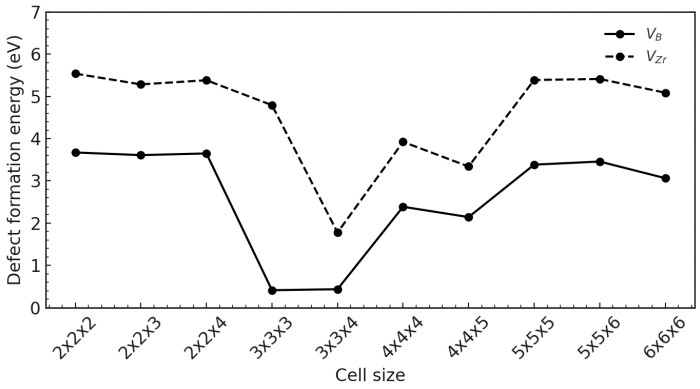


Figure 5: Defect formation energy as a function of supercell size for boron and zirconium vacancies.

zirconium vacancies. The same general trend can be seen as in Figure 5, where intermediate-size cells between 2x2x4 and 4x4x4 show smaller charge deviations.

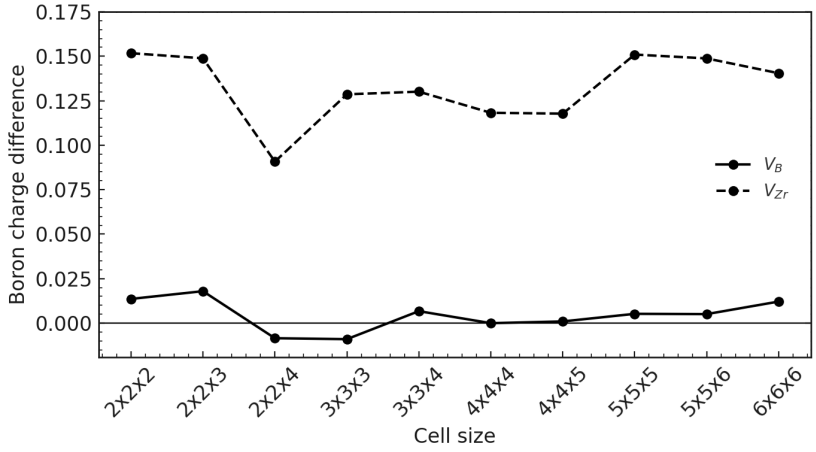


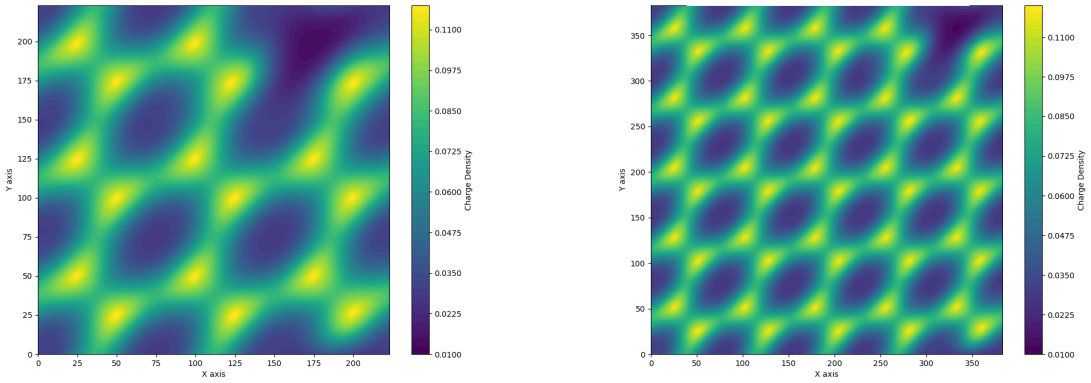
Figure 6: Boron charge difference in pristine ZrB_2 for boron and zirconium vacancies, plotted against supercell size.

Figure 7 shows the spatial distribution of charge in supercells with a boron vacancy. A clear localized charge hole can be seen in the top right of both plots. In the 3×3×3 cell, this defect region takes up a larger portion of the cell compared to the 5×5×5 case. That means the defect in the smaller cell interacts more strongly with its surroundings, possibly disturbing nearby atoms and artificially lowering the formation energy. In contrast, the defect in the larger cell is more isolated.

Based on this, we can say that charge localization influences the defect formation energy. While it may not fully explain the 3 eV difference between the 5x5x5 and 3x3x3 cells, it's likely that other factors are also involved. The 5x5x5 cell appears to be a reasonable choice for the rest of this project.

The formation energies of the boron and zirconium vacancies were calculated using Equation 6, with the chemical potentials taken from bulk boron and zirconium. The resulting values are shown in Table 2. These results show that boron vacancies form more easily than zirconium vacancies, since their formation energy is lower. This agrees with the idea that zirconium atoms are more strongly bound, and their sublattice is more metallic [19].

An inspection of the relaxed structures reveals that both vacancy types perturb the lattice in distinct ways, though the overall distortions remain modest. For the boron vacancy (V_B), Zr atoms



(a) (b)

Figure 7: (a) Localized charge density in a 3x3x3 cell of ZrB_2 with a boron vacancy. (b) Same, but in a 5x5x5 cell.

Table 2: Defect formation energies of intrinsic vacancies in ZrB_2.

Defect Type	Formation Energy (eV)
V_B	3.38
V_{Zr}	5.39

contract slightly toward the defect site, with nearest-neighbour bond lengths decreasing by at most ∼0.05 Å. This is accompanied by a small out-of-plane rumpling of the surrounding atoms, with maximum displacements of about 0.046 Å for B and 0.044 Å for Zr. In contrast, the zirconium vacancy (V_{Zr}) primarily affects the boron sublattice, inducing a weaker but measurable corrugation (∼0.006–0.018 Å on average for B and Zr, respectively). Overall, the mean bond lengths differ from the pristine values by less than 0.001 Å, indicating that while the defects create local distortions, the global lattice parameters remain essentially unchanged. For completeness, the full set of bond statistics and rumpling values is provided in Appendix 7.

These relaxations are also reflected in the charge distribution. Bader charge analysis shows that for V_B, the nearest-neighbor Zr atoms lose on average about 0.2 e^- compared to the pristine structure, while the surrounding B atoms change only slightly (about +0.02 e^-). For V_{Zr}, the nearest B atoms gain on average +0.17 e^- each, showing that they hold more electronic charge when the Zr atom is missing. Atoms further away from the defect remain essentially unchanged, which confirms that the charge redistribution is strongly localized around the vacancy site.

Table 3: Bader charge shifts $\Delta q = q^{(\mathrm{defect})} - q^{(\mathrm{pristine})}$ for atoms near intrinsic vacancies in ZrB_2. Nearest neighbours (NN) are the atoms in the first coordination shell around the vacancy; Far denotes atoms ≥ second shell. Negative values indicate a reduction in Bader electron count (more positive), positive values an increase (more negative).

Defect	NN (first shell)		Far (≥ second shell)	
	Δq_{Zr} (e)	Δq_{B} (e)	Δq_{Zr} (e)	Δq_{B} (e)
V_B	−0.20	+0.02	0.00	0.00
V_{Zr}	0.00	+0.17	0.00	0.00

When compared to literature, the calculated formation energies agree well with earlier reports for bulk ZrB_2, where V_B values of about 3–3.5 eV and V_{Zr} values of about 5–6 eV have been found [19, 27]. Similar trends are also seen in other transition-metal diborides, such as TiB_2 and HfB_2, where vacancies on the metal site are always harder to form and lead to stronger changes in the lattice [9, 10]. This

suggests that boron vacancies are generally easier to form than metal vacancies in these materials, no matter which transition metal is involved.

A density of states (DOS) analysis gives more insight into how these vacancies affect the electronic structure. Boron vacancies introduce localized states close to the Fermi level, which slightly changes the metallic character, but not in a way that destroys conductivity. Zirconium vacancies, however, lead to a noticeable reduction in states at the Fermi level and create defect-related states deeper in the energy spectrum. This suggests some rearrangement in bonding in figure 8

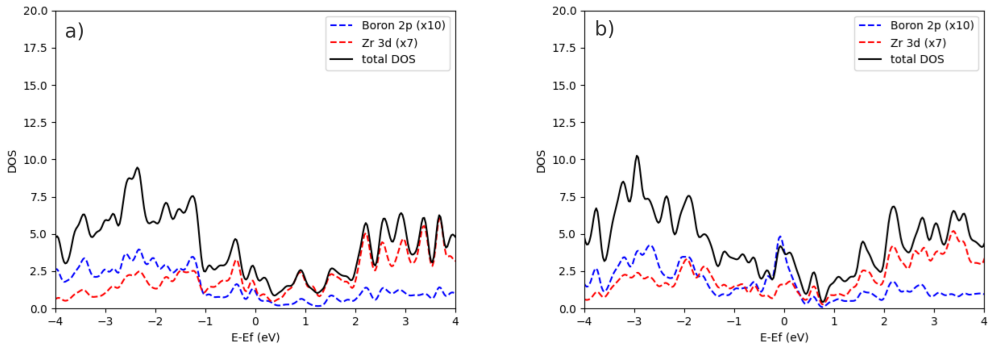


Figure 8: a) Partial DOS of ZrB_2 with a zirconium vacancy. b) Partial DOS with a boron vacancy.

To summarize, boron vacancies are more likely to form, based on their lower formation energy. Still, both vacancy types have noticeable effects on the structure and electronic behavior of ZrB2. From a thermodynamic perspective, the equilibrium concentration of vacancies can be described by

$$n_d \approx N \exp\left(-\frac{\Delta H}{k_B T}\right), \tag{16}$$

where N is the number of possible defect sites, ΔH the defect formation energy, k_B Boltzmann's constant, and T the temperature. This exponential dependence means that even relatively small differences in formation energy translate into large differences in defect concentration. Since boron vacancies have a lower formation energy (~ 3.4 eV) compared to zirconium vacancies (~ 5.4 eV), they will occur at higher concentrations under the same conditions. Thus, while both types of vacancies are possible, boron vacancies are expected to dominate the defect population in ZrB2.

3.3 Adsorption of O, H, and N

We investigated how common extrinsic impurities, oxygen, hydrogen, and nitrogen, interact with the surface of ZrB_2. These elements are relevant because they are often present during synthesis or in operational environments, as they are among the most abundant in the atmosphere. In addition, many two-dimensional materials are known to be unstable under ambient conditions, where exposure to oxygen, moisture, or other reactive species can degrade their structural and electronic properties [36]. This makes it important to understand how such impurities interact with ZrB_2.

To study hydrogen adsorption, seven possible sites on the ZrB_2 surface were tested, as shown in Figure 9. The three most favorable sites, energetically, were found to be site 2, site 5, and site 7. Table 4 shows the formation energies for all seven sites. The negative formation energies for sites 2, 5, and 7 indicate that hydrogen binds most strongly at these locations, whereas adsorption at the other sites is energetically less favorable.

For oxygen and nitrogen, only the three most favorable hydrogen adsorption sites were considered. Oxygen shows negative formation energies at sites 2 and 7, which again indicates that it can adsorb spontaneously. Nitrogen, however, does not show favorable adsorption at any of the sites tested, as all energies are positive. The results for oxygen agree with earlier theoretical studies [37], and experimental reports also suggest oxygen tends to contaminate ZrB_2 during synthesis [38].

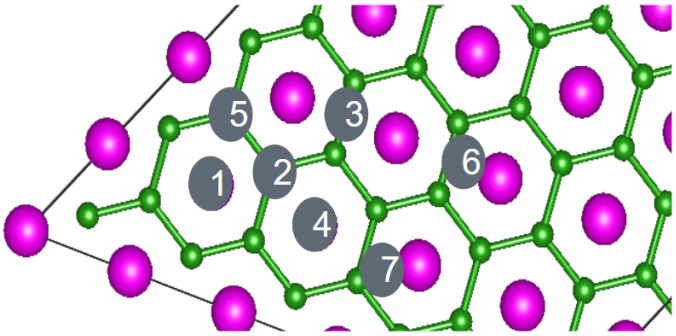


Figure 9: The seven adsorption sites tested for H_i in ZrB_2. The purple atoms are Zr and the green atoms are B.

Table 4: Adsorption energies (eV) for hydrogen at different adsorption sites in ZrB_2.

Site	Adsorption Energy (eV)
Site 1	0.92
Site 2	-0.43
Site 3	0.64
Site 4	0.92
Site 5	-0.31
Site 6	0.64
Site 7	-0.43

The decision to restrict oxygen and nitrogen to the three most favorable hydrogen sites was made to balance accuracy with computational efficiency. Since a full site scan had already been carried out for hydrogen, it seemed reasonable to assume that the less favorable sites would also be less relevant for oxygen and nitrogen. However, this choice introduces limitations, and a more complete study would require testing all possible adsorption sites.

Table 5: Adsorption energies (eV) for nitrogen and oxygen adsorption at the three most favorable sites in ZrB_2.

Site	N_i	O_i
Site 2	2.74	-0.54
Site 5	3.11	0.38
Site 7	2.75	-0.54

The relaxed supercell structures with adsorbed H, O, and N atoms are shown in Appendix A.1, where the positions of the added atoms can be seen clearly.

3.4 Copper Dopant

Copper is a relevant impurity because it can substitute for zirconium or boron atoms in the lattice, or occupy interstitial positions. Such contamination may occur during high-temperature synthesis or processing. For example, copper has been shown to wet and infiltrate ZrB_2 under controlled conditions, indicating that it can readily interact with the ceramic matrix during sintering or composite fabrication [39]. In addition, residual metallic impurities such as copper are known to influence the electrical resistivity of ZrB_2 ceramics, underlining the sensitivity of their electronic properties to trace contamination [40].

Copper is a relevant impurity because it could substitute for zirconium or boron, or occupy interstitial sites, especially under Cu-rich or Zr-deficient synthesis conditions. In related systems, copper doping has been shown to significantly affect material properties: for example, Cu substitution in layered materials such as $ZrSe_2$ induces an electron-doping effect that drives a semiconductor-to-metal

transition [41]. Similarly, substitution of transition metals into ZrB_2 (e.g. Fe, Co, Ni) has demonstrated enhanced catalytic performance in reactions like the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) [42].

From our simulations, copper prefers to substitute on zirconium sites, where it gives a negative formation energy of -0.57 eV, which means the substitution is energetically favorable. However, copper does not easily replace boron, as the formation energy is much higher, around 2.50 eV, making this substitution unlikely.

Of the two substitutional configurations tested, copper incorporation is more favorable on zirconium sites than on boron sites. In relation to cation substitution, occupation of boron sites is therefore less energetically favorable. This indicates that copper is more likely to substitute zirconium rather than boron under the chemical potentials considered.

The relaxed structure of ZrB_2 with a copper substitutional atom is also provided in Appendix A.1, illustrating the local distortion around the impurity site

3.5 High-Energy Photon Transmission

To evaluate whether ZrB_2 is suitable for applications that require transparency to high-energy photons, we computed the dielectric function and calculated the photon transmission for both pristine and defective structures. Specifically, we looked at the most energetically stable defects from earlier parts of the study. The real and imaginary parts of the dielectric function at high photon energies were extracted and are listed in Table 6.

Configuration	Re(ϵ)	Im(ϵ)	Transmittance 50 nm thickness
Pristine	0.9948	0.000058	0.999
V_{Zr}	0.9947	0.000059	0.999
V_{B}	0.9931	0.000077	0.998
H_i	0.9947	0.000059	0.998
O_i	0.9950	0.000056	0.999
$\mathrm{Cu}_{\mathrm{Zr}}$	0.993512	0.000072	0.998

Table 6: Real, imaginary parts of the dielectric function at photon energies of 92 eV for pristine and defective ZrB_2 structures.

The data shows that all the tested structures have a real part of the dielectric function very close to one, and an imaginary part near zero. This indicates the material remains highly transparent at EUV frequencies. Using Equations 11 and 12, we estimated that a 50 nm thick film of ZrB_2 would transmit about 99% of light with a photon energy of 92 eV , even when defects are present, such as vacancies, adsorbates, or dopants.Pellicle thicknesses reported in the literature typically range from about 10 to 80 nm, depending on the material system and transmission requirements [43, 44]. A thickness of 50 nm is therefore taken here as a representative value.

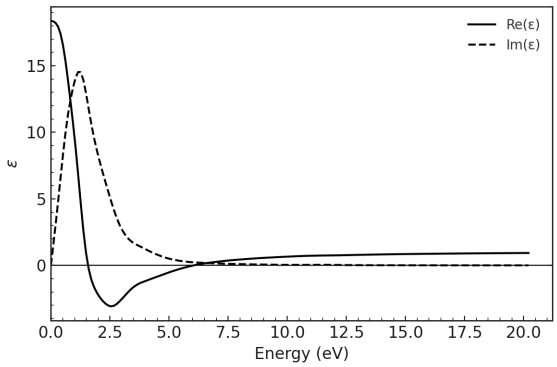
Among the different cases, oxygen adsorption caused a slight increase in the real part of the dielectric function by about 0.0002 and a decrease in the imaginary part by roughly 0.000002 compared to the pristine structure. This corresponds to a small improvement in transparency. In contrast, boron vacancies lowered the real part by approximately 0.0017 and increased the imaginary part by about 0.000019, which makes them slightly worse for transmission. However, these changes remain very small, and the material still shows excellent overall performance.

In general, these results show that ZrB_2 keeps excellent transparency to high-energy photons even with typical point defects. This supports its potential use in optical systems operating in the EUV range. To confirm this, future experiments are needed. It would also be useful to run more simulations at higher defect concentrations to see whether more noticeable effects appear. Finally, oxidation products like ZrO_2 and B_2O_3 [45] should be studied, since they could affect the real-world optical performance of the material when exposed to air or other reactive environments.

3.6 Optical Properties

The interaction of a material with light is governed by its frequency-dependent dielectric function, $\epsilon(\omega)$, which describes the response of electrons to external electromagnetic fields. From it, several measurable quantities can be derived, such as reflectivity, absorption, and the electron energy loss spectrum (EELS). These functions provide direct insight into how defects or impurities affect the underlying electronic structure and, consequently, the performance of the material in practical applications.

The optical response of pristine ZrB_2 is shown in Figures 10a and **??**. The real part of the dielectric function, $\epsilon_1(\omega)$, takes a large positive value at low photon energies, reflecting strong metallic screening. The imaginary part, $\epsilon_2(\omega)$, is finite at low energies, consistent with intraband excitations typical of metallic systems. The corresponding EELS shows a clear plasmon resonance at around 6.5 eV, in good agreement with earlier studies [46].



(a) Real (ϵ_1) and imaginary (ϵ_2) parts of the dielectric function of pristine ZrB_2.

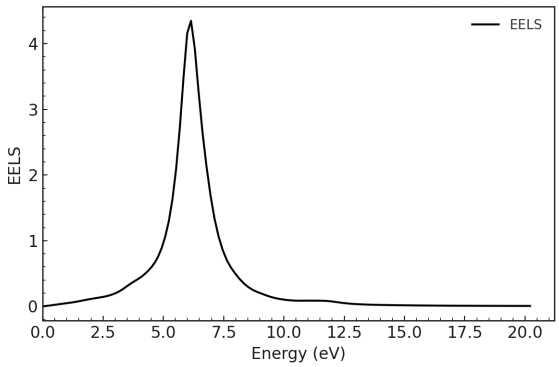
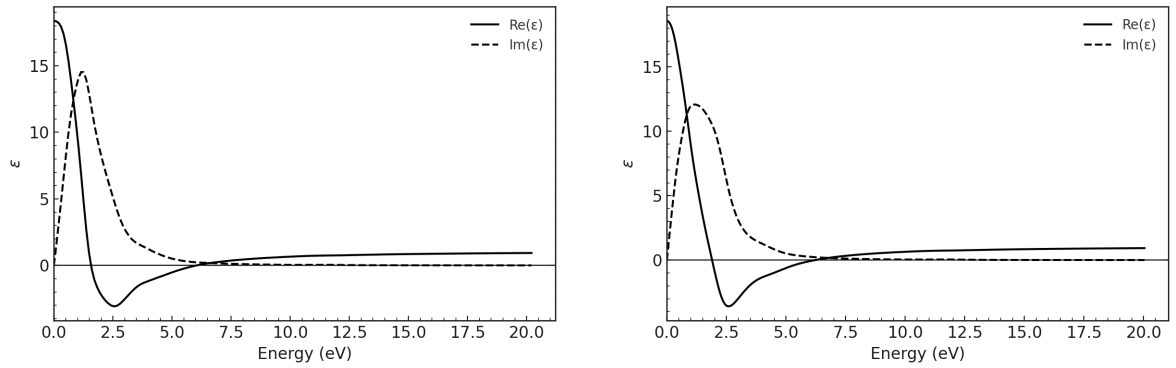


Figure 10: Optical properties of pristine ZrB_2: (a) dielectric function and (b) electron energy loss spectrum (EELS), showing a plasmon peak at ~ 6.5 eV.

The introduction of intrinsic defects alters this picture. Figures 11 and 12 show the dielectric function and EELS for boron and zirconium vacancies. Boron vacancies reduce the magnitude of ϵ_2 slightly, which lowers absorption, but the plasmon resonance remains close to that of the pristine case. Zirconium vacancies, however, have a stronger effect: both ϵ_1 and ϵ_2 are reduced, and the plasmon intensity is dampened. Since zirconium provides most of the conduction electrons, removing it disrupts the metallic screening and leads to weaker collective oscillations. This confirms that zirconium vacancies are more disruptive to the electronic structure than boron vacancies.

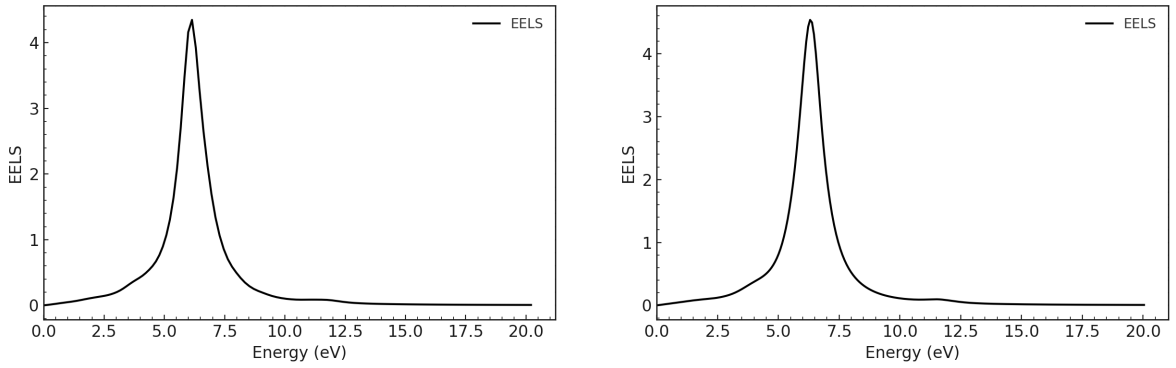
Extrinsic adsorption also modifies the optical response, though in different ways. The dielectric functions with adsorbed hydrogen and oxygen are shown in Figure 13. Hydrogen adsorption produces only minor changes compared to the pristine case, with the plasmon peak position remaining nearly the same. Oxygen adsorption, on the other hand, causes a more pronounced effect: ϵ_2 is suppressed at low energies, and the plasmon resonance shifts downward by about 0.2−0.3 eV, as seen in Figure 14. This shift can be linked to the strong hybridization of oxygen $2p$ states with zirconium $4d$ states, which alters the conduction electron density and weakens collective oscillations. These observations are consistent with the fact that oxygen readily contaminates ZrB_2 surfaces and can significantly change its electronic response [38].

Finally, copper substitution at a zirconium site was investigated. The results, shown in Figure 15, reveal a small increase in ϵ_2 at low energies and a slight shift of the plasmon resonance compared to pristine ZrB_2. This suggests that copper perturbs the metallic bonding environment but does not fundamentally change the collective excitations. Similar observations have been reported in studies of copper-modified diborides, where doping was used to tune surface activity for catalysis [**?**]. Here, the main implication is that while Cu incorporation introduces small additional losses, the overall metallic



(a) (b)

Figure 11: Real and imaginary parts of the dielectric function of ZrB_2 with (a) a boron vacancy, and (b) a zirconium vacancy.



(a) (b)

Figure 12: EELS spectra of ZrB_2 with (a) boron vacancy and (b) zirconium vacancy.

character remains intact.

Overall, these results demonstrate that the optical response of ZrB_2 is robust against many dilute point defects, with only moderate changes in dielectric function and plasmon spectra. Zirconium vacancies and oxygen adsorption represent the strongest perturbations, while hydrogen adsorption and copper substitution have comparatively minor effects. This highlights the central role of zirconium-derived conduction states in governing the dielectric response and the sensitivity of ZrB_2 to oxygen contamination.

4 Conclusion

This thesis explored the potential of ZrB_2 for high-energy photon applications using density functional theory (DFT). As an ultra-high temperature ceramic, ZrB_2 combines a high melting point with strong chemical and mechanical stability, which makes it a good candidate for use in extreme environments and optoelectronic systems [47, 13, 11].

To study how defects influence its behavior, both intrinsic and extrinsic point defects were added to the material. Among all cases, oxygen and hydrogen adsorption were the most energetically favorable, with formation energies of $-0.54\,\text{eV}$ and $-0.43\,\text{eV}$, respectively. In contrast, nitrogen adsorption ($2.74\,\text{eV}$) and vacancy defects—$3.38\,\text{eV}$ for boron and $5.39\,\text{eV}$ for zirconium—were much less likely to occur under typical conditions, which aligns with earlier work [37, 38]. Copper was also tested as

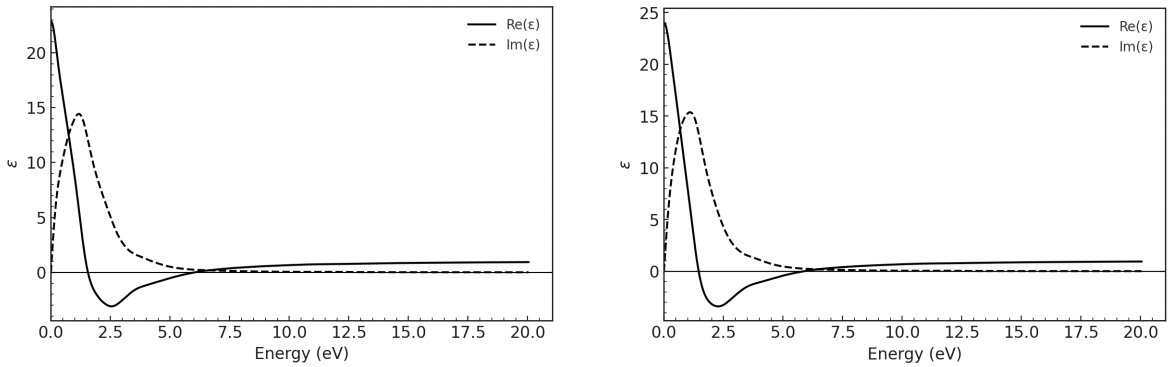


Figure 13: Real (ϵ_1) and imaginary (ϵ_2) parts of the dielectric function of ZrB_2 with (a) hydrogen and (b) oxygen adsorption as a function of photon energy.

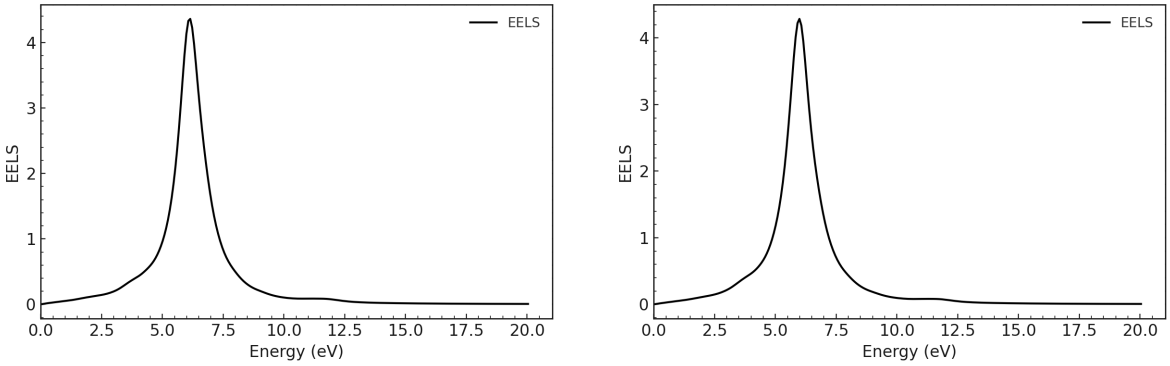


Figure 14: Calculated EELS of ZrB_2 with (a) hydrogen and (b) oxygen adsorption, showing a plasmon peak shift of approximately 0.2−0.3 eV to lower energies, more pronounced for oxygen.

a dopant, and it was found that substitution on zirconium sites is energetically possible (−0.57 eV), while substitution on boron sites is not (2.50 eV). This suggests that copper might be incorporated into ZrB_2 in zirconium-poor, copper-rich environments.

Electronic structure analysis using the partial density of states (PDOS) showed that pristine ZrB_2 remains metallic even when vacancy defects are introduced. Further investigation into the PDOS of other defect types could give more insight into how defect engineering might tune its electronic properties.

The optical properties were also studied using the dielectric function and electron energy loss spectrum (EELS). Pristine ZrB_2 had a strong plasmon peak around 6 eV, which is linked to collective electron oscillations and is typical for good metallic and plasmonic materials [46]. When defects were introduced, only small changes were seen. The biggest shift came from oxygen adsorption, which caused the plasmon peak to move down by about 0.2−0.3 eV, suggesting a slight drop in free carrier density and a change in screening behavior. This could affect performance in highly sensitive plasmonic applications.

Lastly, the EUV transmission of a 50 nm thick ZrB_2 film was estimated for both pristine and defected structures. In all cases, the transmission was about 99%. These results make a strong case for using ZrB_2 in future high-energy optical applications, especially where transparency and durability are both important.

Going forward, experimental work will be needed to confirm these computational results. It would also be useful to look at the effect of higher concentrations of oxygen and hydrogen, as well as common oxidation products like ZrO_2 and B_2O_3 [45], which are likely to form in real environments. This could

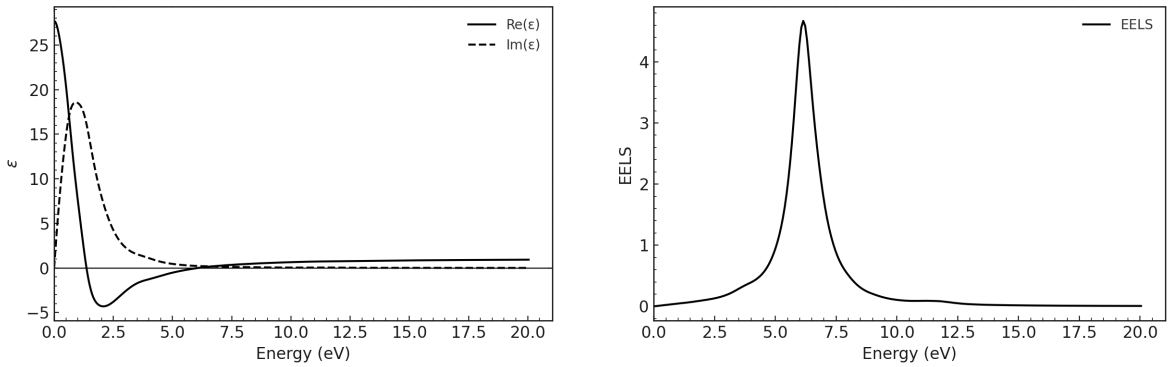


Figure 15: Optical properties of ZrB_2 with a copper dopant substituting a zirconium atom: (a) real and imaginary parts of the dielectric function, (b) EELS showing a slight shift in the plasmon peak compared to pristine ZrB_2.

help determine how robust and practical ZrB_2 really is for long-term use.

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Appendix

A Extra pictures and tables

A.1 Structures

This section provides visualizations of the relaxed supercells with different defects. These complement the numerical analysis of bond lengths and rumpling in Appendix 7.

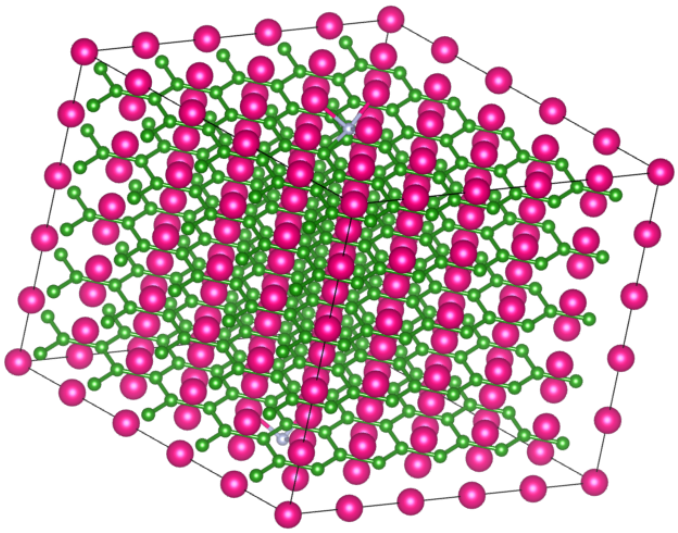

Figure 16: Relaxed structure of ZrB_2 with a nitrogen atom in grey in the middle.

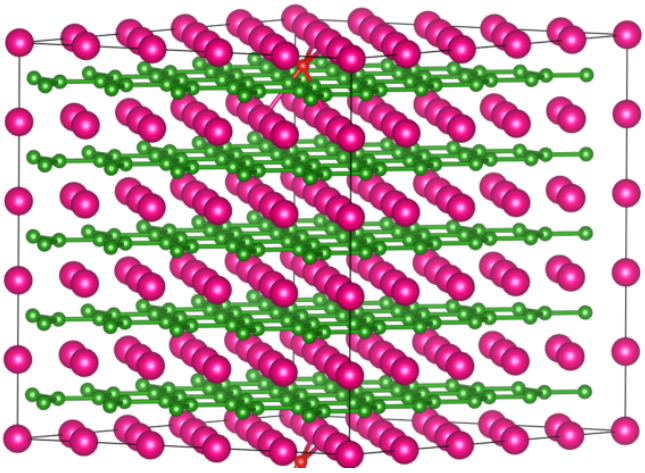

Figure 17: Relaxed structure of ZrB_2 with an oxygen atom in red.

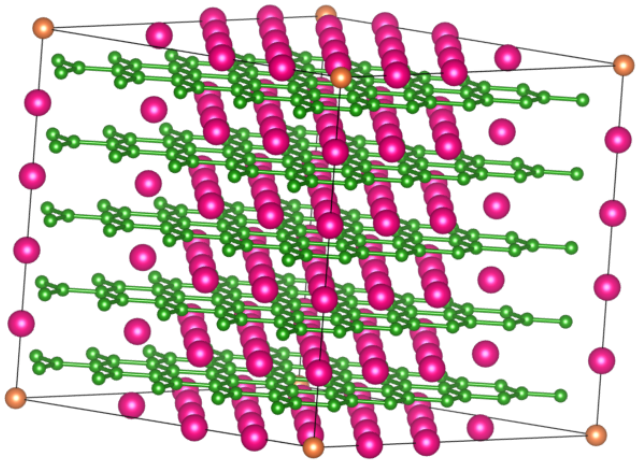

Figure 18: Relaxed structure of ZrB_2 with a copper substitutional impurity in orange. In the picture you see 8 copper atoms, this is a prurely visual and a byproduct of the program VESTA. The analysis was done with only one added copper atom, which can be checked in the POSCAR file of appendix B.

A.2 Bader analysis

B Program and input files

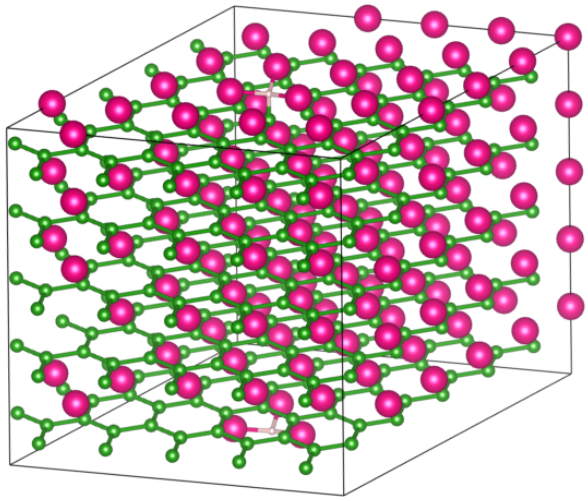

Figure 19: Relaxed structure of ZrB_2 with a hydrogen atom in light pink.

This appendix includes the key Python scripts and structural input files used in the simulations and analysis.

bader_an.py

```
import numpy as np
import os

def read_charges(file_path):
    charges = []
    with open(file_path, 'r') as file:
        lines = file.readlines()
        for line in lines:
            if line.strip() and not line.startswith(("#", "-")):  # Skip
                headers and empty lines
                parts = line.split()
                charges.append(float(parts[4]))  # CHARGE is the 5th column
    return charges

def calculate_charge_difference(file1, file2):
    charges1 = read_charges(file1)
    charges2 = read_charges(file2)

    if len(charges1) != len(charges2):
        raise ValueError("Files have different number of charges")

    charge_differences = np.array(charges2) - np.array(charges1)
    return charge_differences

def main():
    file1 = 'ACF_B.dat'  # Replace with your first .dat file path
    file2 = 'ACF_P.dat'  # Replace with your second .dat file path

    charge_differences = calculate_charge_difference(file1, file2)
```

Table 7: First-shell bond statistics (Å) and per-species rumpling (Å) from. Deltas are relative to pristine means.

System	Pair	min	median	mean	max	Δmean
Pristine	B–B	1.828770	1.828771	1.828771	1.828773	–
Pristine	B–Zr	2.549365	2.549366	2.549366	2.549368	–
Pristine	Zr–Zr	3.167524	3.167525	3.267924	3.552389	–
V_B	B–B	1.781212	1.828421	1.827775	1.842283	−0.0010
V_B	B–Zr	2.456586	2.549400	2.549244	2.572403	−0.00012
V_B	Zr–Zr	3.156385	3.168535	3.266971	3.582640	−0.00095
V_{Zr}	B–B	1.803758	1.828953	1.828773	1.839490	+0.000002
V_{Zr}	B–Zr	2.537266	2.549480	2.549499	2.564534	+0.000132
V_{Zr}	Zr–Zr	3.136170	3.170884	3.268322	3.557284	+0.000398
Rumpling ($\lvert z - \bar{z} \rvert$, Å) **per species**						
Pristine	B	mean = 0.000000, max = 0.000000				
Pristine	Zr	mean = 0.000000, max = 0.000000				
V_B	B	mean = 0.021517, max = 0.046130				
V_B	Zr	mean = 0.017932, max = 0.044088				
V_{Zr}	B	mean = 0.003289, max = 0.005571				
V_{Zr}	Zr	mean = 0.006844, max = 0.018477				

```
    for i, diff in enumerate(charge_differences, start=1):
        with open('bade_diff.txt', 'w') as file:
            file.write(f"Atom␣{i}:␣Charge␣difference␣=␣{diff:.6f}")

if __name__ == "__main__":
    main()
```

Listing 1: Script for analyzing or generating data for Bader charge calculations.

bader_cube.py

```
from ase.build import molecule
from ase.io import write
from ase.units import Bohr
from gpaw import GPAW
from gpaw.analyse.hirshfeld import HirshfeldPartitioning
import numpy as np
from gpaw import GPAW, PW, FermiDirac
from ase.io import vasp
from ase import Atoms
from ase.optimize import BFGS
from ase.optimize import QuasiNewton
from ase.visualize import view
from ase.io import read,write
from ase.constraints import StrainFilter
from ase.io import Trajectory
import os

folder_path_B = 'CONTCAR_B/'
cube_output_B = 'cube_B/'

folder_path_pris = 'pristine/'
cube_output_pris = 'cube_pris/'

file_list_B = os.listdir(folder_path_B)

k = 5
```

```
for filename in file_list_B:

    if k == 0:
        k = 1

    full_path = os.path.join(folder_path_B, filename)
    zr = read(filename=full_path)

    calc = GPAW(mode=PW(650),
            xc='RPBE',
            kpts=(k,k,k),
            occupations=FermiDirac(0.01))

    zr.calc=calc
    zr.get_potential_energy()
    rho = zr.calc.get_all_electron_density(gridrefinement=4)
    base_filename = os.path.splitext(filename)[0].split('_')[-1]
    cube_filename = os.path.join(cube_output_B, f'{base_filename}.cube')
    write(cube_filename, zr, data=rho * Bohr**3)
    k -= 1

file_list_pris = os.listdir(folder_path_pris)

l = 5
for filename in file_list_pris:

    if l == 0:
        l = 1

    full_path = os.path.join(folder_path_pris, filename)
    zr = read(filename=full_path)

    calc = GPAW(mode=PW(650),
            xc='RPBE',
            kpts=(l,l,l),
            occupations=FermiDirac(0.01))

    zr.calc=calc
    zr.get_potential_energy()
    rho = zr.calc.get_all_electron_density(gridrefinement=4)
    base_filename = os.path.splitext(filename)[0].split('_')[-1]
    cube_filename = os.path.join(cube_output_pris, f'{base_filename}.cube')
    write(cube_filename, zr, data=rho * Bohr**3)
    l -= 1
```

Listing 2: Script for analyzing or generating data for Bader charge calculations.

read.py

```
import pandas as pd
import re
import numpy as np
import os
from openpyxl import Workbook
from openpyxl import load_workbook

wb = load_workbook(filename='bader.xlsx')
ws = wb.active

file_path_B = 'ACF_B_5.dat'
```

```
file_path_Zr = 'ACF_Zr_5.dat'
file_path_P = 'ACF_P_5.dat'

Zr_charges_B = []
B_charges_B = []

Zr_charges_P = []
B_charges_P = []

Zr_charges_Zr = []
B_charges_Zr = []

with open(file_path_B, 'r') as file:
    lines = file.readlines()
    for line in lines:
        if line.strip() and not line.startswith(("#", "-")):  # Skip headers
            and empty lines
            parts = re.split(r'\s+', line.strip())
            if len(parts) > 4:  # Ensure there are enough parts in the line
                charge = float(parts[4])
                if charge > 30:
                    Zr_charges_B.append(charge)
                else:
                    B_charges_B.append(charge)

std_Zr_charges_B = np.std(Zr_charges_B)
std_B_charges_B = np.std(B_charges_B)
ws.cell(row=3, column=2, value=std_Zr_charges_B)
ws.cell(row=3, column=3, value=std_B_charges_B)

# print(f"Zr Charges: {Zr_charges}")
# print(f"B Charges: {B_charges}")
print(f"Standard␣Deviation␣of␣Zr␣Charges:␣{std_Zr_charges_B:.6f}")
print(f"Standard␣Deviation␣of␣B␣Charges:␣{std_B_charges_B:.6f}")

with open(file_path_P, 'r') as file:
    lines = file.readlines()
    for line in lines:
        if line.strip() and not line.startswith(("#", "-")):  # Skip headers
            and empty lines
            parts = re.split(r'\s+', line.strip())
            if len(parts) > 4:  # Ensure there are enough parts in the line
                charge = float(parts[4])
                if charge > 30:
                    Zr_charges_P.append(charge)
                else:
                    B_charges_P.append(charge)

std_Zr_charges_P = np.std(Zr_charges_P)
std_B_charges_P = np.std(B_charges_P)
ws.cell(row=3, column=6, value=std_Zr_charges_P)
ws.cell(row=3, column=7, value=std_B_charges_P)

# print(f"Zr Charges: {Zr_charges}")
# print(f"B Charges: {B_charges}")
print(f"Standard␣Deviation␣of␣Zr␣Charges:␣{std_Zr_charges_P:.6f}")
print(f"Standard␣Deviation␣of␣B␣Charges:␣{std_B_charges_P:.6f}")

with open(file_path_Zr, 'r') as file:
    lines = file.readlines()
    for line in lines:
```

```
        if line.strip() and not line.startswith(("#", "-")):  # Skip headers
            and empty lines
            parts = re.split(r'\s+', line.strip())
            if len(parts) > 4:  # Ensure there are enough parts in the line
                charge = float(parts[4])
                if charge > 30:
                    Zr_charges_Zr.append(charge)
                else:
                    B_charges_Zr.append(charge)

std_Zr_charges_Zr = np.std(Zr_charges_Zr)
std_B_charges_Zr = np.std(B_charges_Zr)
ws.cell(row=3, column=4, value=std_Zr_charges_P)
ws.cell(row=3, column=5, value=std_B_charges_P)


ws.cell(row=3, column=8, value=std_Zr_charges_B - std_Zr_charges_P)
ws.cell(row=3, column=9, value=std_B_charges_B - std_B_charges_P)
ws.cell(row=3, column=10, value=std_Zr_charges_Zr - std_Zr_charges_P)
ws.cell(row=3, column=11, value=std_B_charges_Zr - std_B_charges_P)
# print(f"Zr Charges: {Zr_charges}")
# print(f"B Charges: {B_charges}")
print(f"Standard␣Deviation␣of␣Zr␣Charges:␣{std_Zr_charges_Zr:.6f}")
print(f"Standard␣Deviation␣of␣B␣Charges:␣{std_B_charges_Zr:.6f}")


print(f"Diff␣std␣B␣and␣P␣for␣Zr␣atom:␣{std_Zr_charges_B␣-␣std_Zr_charges_P:.6f
    }")
print(f"Diff␣std␣B␣and␣P␣for␣B␣atom:␣{std_B_charges_B␣-␣std_B_charges_P:.6f}")

print(f"Diff␣std␣Zr␣and␣P␣for␣Zr␣atom:␣{std_Zr_charges_Zr␣-␣std_Zr_charges_P
    :.6f}")
print(f"Diff␣std␣Zr␣and␣P␣for␣B␣atom:␣{std_B_charges_Zr␣-␣std_B_charges_P:.6f}
    ")

wb.save("bader.xlsx")
```

Listing 3: General simulation or analysis script.

bulk.py

```
from ase import Atoms
from ase.lattice.hexagonal import Hexagonal
import matplotlib.pyplot as plt

from gpaw import GPAW, PW, FermiDirac
from gpaw.response.df import DielectricFunction
from gpaw.mpi import world
from gpaw.bztools import find_high_symmetry_monkhorst_pack
from ase.io import read
from ase import Atoms
from ase.build import bulk
from gpaw import GPAW
from gpaw import PW
from gpaw.occupations import FermiDirac
import numpy as np
from ase.build import find_optimal_cell_shape
from ase.build import make_supercell
from ase.build import bulk
from gpaw import GPAW, PW, FermiDirac
from ase import Atoms
```

```
from ase.optimize import BFGS
from ase.optimize import QuasiNewton
from ase.lattice.hexagonal import Graphite #set up graphite using ASE
from ase.lattice.hexagonal import Graphene #set up graphene using ASE
from ase.visualize import view
from ase.io import read
from ase.constraints import StrainFilter
from ase.io import Trajectory


zr =  read(filename="POSCAR")

calc = GPAW('v.gpw')

# Assign the loaded calculator to the structure
zr.set_calculator(calc)

calc.diagonalize_full_hamiltonian() #same number of bands as there are atomic
    orbitals
calc.write('gs_zr_vac.gpw', mode='all')
```

Listing 4: General simulation or analysis script.

chem_pot.py

```
import numpy as np
import matplotlib.pyplot as plt
from ase.build import find_optimal_cell_shape
from ase.build import make_supercell
from ase.build import bulk
from gpaw import GPAW, PW, FermiDirac
from ase.io import vasp
from ase import Atoms
from ase.optimize import BFGS
from ase.optimize import QuasiNewton
from ase.lattice.hexagonal import Graphite #set up graphite using ASE
from ase.lattice.hexagonal import Graphene #set up graphene using ASE
from ase.visualize import view
from ase.io import read,write
from ase.constraints import StrainFilter
from ase.io import Trajectory



from ase import Atoms

n2 = Atoms('Cu', [(0, 0, 0)])
n2.center(vacuum=5)


calc = GPAW(mode=PW(650),
            xc = "RPBE",
            occupations=FermiDirac(0.01))

n2.calc = calc

opt = BFGS(n2)
opt.run(fmax=0.01)

chem = n2.get_potential_energy()
```

```
write('CONTCAR', n2) #POSCAR format
with open('defect_energy.txt', 'w') as file:
    file.write(f'Defect Energy: {chem} eV\n')
```

Listing 5: Defines chemical potentials for defect formation energy calculations.

combined.py

```
import numpy as np
from gpaw import GPAW, PW, FermiDirac
from ase.io import vasp
from ase import Atoms
from ase.optimize import BFGS
from ase.optimize import QuasiNewton
from ase.visualize import view
from ase.io import read,write
from ase.constraints import StrainFilter
from ase.io import Trajectory
import os
from openpyxl import Workbook
from openpyxl import load_workbook

wb = load_workbook(filename='B_defect.xlsx')
ws = wb.active

folder_path = 'POSCAR2/'
contcar_output = 'CONTCAR/'
traj_output = 'traj/'
folder_path_pris = 'pristine2/'

file_list = os.listdir(folder_path)
i = 6
k = 1

for filename in file_list:

    if k == 0:
        k = 1

    full_path = os.path.join(folder_path, filename)
    zr = read(filename=full_path)

    calc = GPAW(mode=PW(650),
            xc='RPBE',
            kpts=(k,k,k),
            occupations=FermiDirac(0.01))

    zr.calc=calc

    base_filename = os.path.splitext(filename)[0].split('_')[-1]

    calcname = f'zr_opt_{base_filename}'
    traj_filename = os.path.join(traj_output, f'{base_filename}.traj')
    contcar_filename = os.path.join(contcar_output, f'CONTCAR_{base_filename}'
        )

    opt=BFGS(zr,trajectory=traj_filename)
    opt.run(fmax=0.01)

    E_defect = zr.get_potential_energy()
    ws.cell(row=i, column=1, value=base_filename)
```

```
    ws.cell(row=i, column=2, value=E_defect)
    write(contcar_filename, zr) #POSCAR format\
    i = i + 1
    k = k - 1
    wb.save("B_defect.xlsx")


file_list_prist = os.listdir(folder_path_pris)
j = 7

for filename in file_list_prist:
    full_path = os.path.join(folder_path, filename)
    zr = read(filename=full_path)

    calc = GPAW(mode=PW(650),
            xc='RPBE',
            kpts=(k,k,k),
            occupations=FermiDirac(0.01))

    zr.calc=calc
    E_pristine = zr.get_potential_energy()
    ws.cell(row=i, column=3, value=E_pristine)
    i = i + 1
    wb.save("B_defect.xlsx")
    k = k - 1
```

Listing 6: General simulation or analysis script.

defect.py

```
import numpy as np
from gpaw import GPAW, PW, FermiDirac
from ase.io import vasp
from ase import Atoms
from ase.optimize import BFGS
from ase.optimize import QuasiNewton
from ase.visualize import view
from ase.io import read,write
from ase.constraints import StrainFilter
from ase.io import Trajectory
import os
from openpyxl import Workbook
from openpyxl import load_workbook

wb = load_workbook(filename='B_defect.xlsx')
ws = wb.active

folder_path = 'POSCAR_Zr/'
contcar_output = 'CONTCAR_Zr/'
traj_output = 'traj_Zr/'

file_list = os.listdir(folder_path)
i = 2
k = 5

for filename in file_list:

    if k == 0:
        k = 1

    full_path = os.path.join(folder_path, filename)
```

```
    zr = read(filename=full_path)

    calc = GPAW(mode=PW(650),
            xc='RPBE',
            kpts=(k,k,k),
            occupations=FermiDirac(0.01))

    zr.calc=calc

    base_filename = os.path.splitext(filename)[0].split('_')[-1]

    calcname = f'zr_opt_{base_filename}'
    traj_filename = os.path.join(traj_output, f'{base_filename}.traj')
    contcar_filename = os.path.join(contcar_output, f'CONTCAR_{base_filename}'
        )

    opt=BFGS(zr,trajectory=traj_filename)
    opt.run(fmax=0.01)

    E_defect = zr.get_potential_energy()
    # ws.cell(row=i, column=1, value=base_filename)
    ws.cell(row=i, column=5, value=E_defect)
    write(contcar_filename, zr) #POSCAR format\
    i = i + 1
    k = k - 1
    wb.save("B_defect.xlsx")
```

Listing 7: Script for introducing or analyzing defects.

PDOS.py

```
from gpaw import GPAW, PW,FermiDirac,restart
import matplotlib.pyplot as plt
import numpy as np
from ase.io import read
from ase.io import Trajectory


ldos_B = 10
ldos_Ti =7




calc = GPAW('gpw_B/4x4x5.gpw', txt=None)


ef = calc.get_fermi_level()

energies, ldos = calc.get_orbital_ldos(a=100, npts=2001, angular='2p',width
    =0.1)
plt.plot(energies - ef, ldos*ldos_B,'--', label=f'Boron␣2p␣(x{ldos_B})', color
     = 'blue')
energies, ldos = calc.get_orbital_ldos(a=1, npts=2001, angular='3d',width
    =0.1)
plt.plot(energies - ef, ldos*ldos_Ti,'--', label=f'Zr␣3d␣(x{ldos_Ti})', color
    = 'red' )

# Density of States
slab, calc = restart(f'gpw_B/4x4x5.gpw')
e, dos = calc.get_dos( npts=2001,width=0.1)
```

```
plt.plot(e - ef, dos,label='total␣DOS', color = 'k')
plt.axis([-4, 4,0,20])
plt.title('PDOS/DOS␣ZrB2␣Boron␣vacancy␣4x4x5␣xc=RPBE')
plt.xlabel('E-Ef␣(eV)')
plt.ylabel('DOS')
plt.legend()
plt.savefig(f'PDOS_B/PDOS_4x4x5_Bvac.png')
```

Listing 8: Script for projecting the density of states (PDOS).

plot.py

```
import matplotlib.pyplot as plt
import numpy as np
from scipy.constants import hbar
from scipy.constants import h
from scipy.constants import c


h_con = 4.135667696 * 10 ** (-15)
plt.figure()
d = np.loadtxt('dfpristine.csv', delimiter=',')

e_1 = d[:,3] #Re
e_2 = d[:,4] #Im

#Re and Im part of the Dielectric function

plt.plot(d[:, 0], d[:,4], '-', label=r'$\mathrm{Im}\epsilon(\omega)$')

#plt.axis([10, 30, 0, 10])

plt.xlabel(r'$\omega\;[eV]$')
plt.ylabel(r'$\epsilon$')
plt.savefig('DIEL_F_Im_pris.png')
plt.clf()




plt.plot(d[:, 0], d[:,3], '-', label=r'$\mathrm{Re}\epsilon(\omega)$')

plt.hlines(0, 0, 50, linestyle="dashed")
plt.xlabel(r'$\omega\;[eV]$')
plt.ylabel(r'$\epsilon$')
plt.savefig('DIEL_F_Re2_pris.png')
plt.clf()
```

Listing 9: Script for plotting defect or charge-related data.

pot_en.py

```
import numpy as np
from gpaw import GPAW, PW, FermiDirac
from ase.io import vasp
from ase import Atoms
from ase.optimize import BFGS
from ase.optimize import QuasiNewton
from ase.visualize import view
```

```
from ase.io import read,write
from ase.constraints import StrainFilter
from ase.io import Trajectory
import os
from openpyxl import Workbook
from openpyxl import load_workbook

wb = load_workbook(filename='B_defect.xlsx')
ws = wb.active
folder_path = 'pristine2/'

file_list = os.listdir(folder_path)
i = 7
k = 1

for filename in file_list:
    full_path = os.path.join(folder_path, filename)
    zr = read(filename=full_path)

    calc = GPAW(mode=PW(650),
            xc='RPBE',
            kpts=(k,k,k),
            occupations=FermiDirac(0.01))

    zr.calc=calc
    E_pristine = zr.get_potential_energy()
    ws.cell(row=i, column=3, value=E_pristine)
    i = i + 1
    wb.save("B_defect.xlsx")
```

Listing 10: General simulation or analysis script.

df.py

```
import numpy as np
from gpaw.response.bse import BSE
from gpaw.response.df import DielectricFunction
from gpaw import FermiDirac
from pathlib import Path

from ase.build import bulk
from ase.parallel import paropen, world

ecut = 100
eshift = 0.8
eta = 0.05

df = DielectricFunction(calc='ZrB2-gsresponse.gpw',
    eta=eta,
    ecut=ecut,
    frequencies={'type': 'nonlinear', 'domega0': 0.05},
    nbands = 1000,
    intraband=False,
    hilbert=False,
    nblocks = 128,
    txt='rpa_df.txt',
    integrationmode='tetrahedron␣integration')



df.get_dielectric_function(filename='df1.csv',direction='x')
```

Listing 11: Script for dielectric function or DFT-related calculations.

diel.py

```
from ase import Atoms
from ase.lattice.hexagonal import Hexagonal
import matplotlib.pyplot as plt

from gpaw import GPAW, PW, FermiDirac
from gpaw.response.df import DielectricFunction
from gpaw.mpi import world
from gpaw.bztools import find_high_symmetry_monkhorst_pack
from ase.io import read

#ground state
zr =  read(filename="CONTCAR")

calc = GPAW(mode=PW(650),
        xc='PBE',
        kpts=(2,2,2),
        occupations=FermiDirac(0.01))

zr.calc = calc
zr.get_potential_energy()
calc.write('zr_gs.gpw')

#unoccupied bands

kpts = find_high_symmetry_monkhorst_pack('zr_gs.gpw', density=20.0)
nbands = 1300

responseGS = GPAW('zr_gs.gpw').fixed_density(
    kpts=kpts,
    parallel={'band': 1},
    nbands= nbands,
    convergence={'bands':50}
)

responseGS.get_potential_energy()
responseGS.write('zr_gsresponse.gpw', 'all')

#dielecetric function

df = DielectricFunction(
    'zr_gsresponse.gpw',
    eta=25e-3,
    rate='eta',
    frequencies={'type': 'nonlinear', 'domega0': 0.01},
    integrationmode='tetrahedron␣integration')

df.get_dielectric_function(filename='df1.csv')
df1tetra_w, df2tetra_w = df.get_dielectric_function(direction='x')

df = DielectricFunction(
    'zr_gsresponse.gpw',
    eta=25e-3,
    rate='eta',
    frequencies={'type': 'nonlinear', 'domega0': 0.01})
```

```
df.get_dielectric_function(filename='df2.csv')

df1_w, df2_w = df.get_dielectric_function(direction='x')
omega_w = df.get_frequencies()

plt.figure(figsize=(6, 6))
plt.plot(omega_w, df2tetra_w.real, label='tetra Re')
plt.plot(omega_w, df2tetra_w.imag, label='tetra Im')
plt.plot(omega_w, df2_w.real, label='Re')
plt.plot(omega_w, df2_w.imag, label='Im')
plt.xlabel('Frequency (eV)')
plt.ylabel('$\\varepsilon$')
plt.xlim(0, 20)
plt.ylim(-20, 20)
plt.legend()
plt.tight_layout()
plt.savefig('eps.png', dpi=600)
plt.show()
```

Listing 12: Script for dielectric function or DFT-related calculations.

gs_df.py

```
from ase import Atoms
from ase.build import bulk
from gpaw import GPAW
from gpaw import PW
from gpaw.occupations import FermiDirac
import numpy as np
from ase.build import find_optimal_cell_shape
from ase.build import make_supercell
from ase.build import bulk
from gpaw import GPAW, PW, FermiDirac
from ase import Atoms
from ase.optimize import BFGS
from ase.optimize import QuasiNewton
from ase.lattice.hexagonal import Graphite #set up graphite using ASE
from ase.lattice.hexagonal import Graphene #set up graphene using ASE
from ase.visualize import view
from ase.io import read
from ase.constraints import StrainFilter
from ase.io import Trajectory
from gpaw.mpi import world

from gpaw import GPAW, PW, FermiDirac
from gpaw.response.df import DielectricFunction
from gpaw.mpi import world
from gpaw.bztools import find_high_symmetry_monkhorst_pack

zr =  read(filename="POSCAR")

calc = GPAW(mode=PW(650),
            xc='PBE',
            occupations=FermiDirac(width=0.01),
            kpts={'density': 5},
            parallel={'domain': 1, 'kpt': 1})

zr.calc = calc
zr.get_potential_energy()
calc.write('ZrB2-gs.gpw')
```

```
kpts = find_high_symmetry_monkhorst_pack('ZrB2-gs.gpw', density=5.0)

responseGS = GPAW('ZrB2-gs.gpw').fixed_density(
    kpts=kpts,
    parallel={'band': 1, 'kpt' : 1},
    nbands=600,
    convergence={'bands': 300})

responseGS.get_potential_energy()
responseGS.write('ZrB2␣␣-gsresponse.gpw', 'all')
```

Listing 13: Script for dielectric function or DFT-related calculations.

5x5x5_B_inter POSCAR

```
# Zr1 B2
1.000000
      7.91881165      -13.71578412        0.00000000
      7.91881165       13.71578412        0.00000000
      0.00000000        0.00000000       17.76194030
 Zr  B
   124     251
Cartesian
      0.00000000        0.00000000        0.00000000
      1.58376233       -2.74315682        0.00000000
      3.16752466       -5.48631365        0.00000000
      4.75128699       -8.22947047        0.00000000
      6.33504932      -10.97262730        0.00000000
      1.58376233        2.74315682        0.00000000
      3.16752466        0.00000000        0.00000000
      4.75128699       -2.74315682        0.00000000
      6.33504932       -5.48631365        0.00000000
      7.91881165       -8.22947047        0.00000000
      3.16752466        5.48631365        0.00000000
      4.75128699        2.74315682        0.00000000
      6.33504932        0.00000000        0.00000000
      7.91881165       -2.74315682        0.00000000
      9.50257398       -5.48631365        0.00000000
      4.75128699        8.22947047        0.00000000
      6.33504932        5.48631365        0.00000000
      7.91881165        2.74315682        0.00000000
      9.50257398        0.00000000        0.00000000
     11.08633632       -2.74315682        0.00000000
      6.33504932       10.97262730        0.00000000
      7.91881165        8.22947047        0.00000000
      9.50257398        5.48631365        0.00000000
     11.08633632        2.74315682        0.00000000
     12.67009865        0.00000000        0.00000000
      0.00000000        0.00000000        3.55238806
      1.58376233       -2.74315682        3.55238806
      3.16752466       -5.48631365        3.55238806
      4.75128699       -8.22947047        3.55238806
      6.33504932      -10.97262730        3.55238806
      1.58376233        2.74315682        3.55238806
      3.16752466        0.00000000        3.55238806
      4.75128699       -2.74315682        3.55238806
      6.33504932       -5.48631365        3.55238806
      7.91881165       -8.22947047        3.55238806
      3.16752466        5.48631365        3.55238806
      4.75128699        2.74315682        3.55238806
      6.33504932        0.00000000        3.55238806
```

```
 7.91881165  -2.74315682   3.55238806
 9.50257398  -5.48631365   3.55238806
 4.75128699   8.22947047   3.55238806
 6.33504932   5.48631365   3.55238806
 7.91881165   2.74315682   3.55238806
 9.50257398   0.00000000   3.55238806
11.08633632  -2.74315682   3.55238806
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
```

```
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
```

```
 11.08633632        -0.91438561         1.77619403
 12.67009865        -1.82877122         1.77619403
 12.67009865        -3.65754243         1.77619403
  7.91881165        11.88701290         1.77619403
  7.91881165        10.05824169         1.77619403
  9.50257398         9.14385608         1.77619403
  9.50257398         7.31508486         1.77619403
 11.08633632         6.40069926         1.77619403
 11.08633632         4.57192804         1.77619403
 12.67009865         3.65754243         1.77619403
 12.67009865         1.82877122         1.77619403
 14.25386098         0.91438561         1.77619403
 14.25386098        -0.91438561         1.77619403
  1.58376233         0.91438561         5.32858209
  1.58376233        -0.91438561         5.32858209
  3.16752466        -1.82877122         5.32858209
  3.16752466        -3.65754243         5.32858209
  4.75128699        -4.57192804         5.32858209
  4.75128699        -6.40069926         5.32858209
  6.33504932        -7.31508486         5.32858209
  6.33504932        -9.14385608         5.32858209
  7.91881165       -10.05824169         5.32858209
  7.91881165       -11.88701290         5.32858209
  3.16752466         3.65754243         5.32858209
  3.16752466         1.82877122         5.32858209
  4.75128699         0.91438561         5.32858209
  4.75128699        -0.91438561         5.32858209
  6.33504932        -1.82877122         5.32858209
  6.33504932        -3.65754243         5.32858209
  7.91881165        -4.57192804         5.32858209
  7.91881165        -6.40069926         5.32858209
  9.50257398        -7.31508486         5.32858209
  9.50257398        -9.14385608         5.32858209
  4.75128699         6.40069926         5.32858209
  4.75128699         4.57192804         5.32858209
  6.33504932         3.65754243         5.32858209
  6.33504932         1.82877122         5.32858209
  7.91881165         0.91438561         5.32858209
  7.91881165        -0.91438561         5.32858209
  9.50257398        -1.82877122         5.32858209
  9.50257398        -3.65754243         5.32858209
 11.08633632        -4.57192804         5.32858209
 11.08633632        -6.40069926         5.32858209
  6.33504932         9.14385608         5.32858209
  6.33504932         7.31508486         5.32858209
  7.91881165         6.40069926         5.32858209
  7.91881165         4.57192804         5.32858209
  9.50257398         3.65754243         5.32858209
  9.50257398         1.82877122         5.32858209
 11.08633632         0.91438561         5.32858209
 11.08633632        -0.91438561         5.32858209
 12.67009865        -1.82877122         5.32858209
 12.67009865        -3.65754243         5.32858209
  7.91881165        11.88701290         5.32858209
  7.91881165        10.05824169         5.32858209
  9.50257398         9.14385608         5.32858209
  9.50257398         7.31508486         5.32858209
 11.08633632         6.40069926         5.32858209
 11.08633632         4.57192804         5.32858209
 12.67009865         3.65754243         5.32858209
 12.67009865         1.82877122         5.32858209
 14.25386098         0.91438561         5.32858209
```

```
14.25386098  -0.91438561   5.32858209
 1.58376233   0.91438561   8.88097015
 1.58376233  -0.91438561   8.88097015
 3.16752466  -1.82877122   8.88097015
 3.16752466  -3.65754243   8.88097015
 4.75128699  -4.57192804   8.88097015
 4.75128699  -6.40069926   8.88097015
 6.33504932  -7.31508486   8.88097015
 6.33504932  -9.14385608   8.88097015
 7.91881165 -10.05824169   8.88097015
 7.91881165 -11.88701290   8.88097015
 3.16752466   3.65754243   8.88097015
 3.16752466   1.82877122   8.88097015
 4.75128699   0.91438561   8.88097015
 4.75128699  -0.91438561   8.88097015
 6.33504932  -1.82877122   8.88097015
 6.33504932  -3.65754243   8.88097015
 7.91881165  -4.57192804   8.88097015
 7.91881165  -6.40069926   8.88097015
 9.50257398  -7.31508486   8.88097015
 9.50257398  -9.14385608   8.88097015
 4.75128699   6.40069926   8.88097015
 4.75128699   4.57192804   8.88097015
 6.33504932   3.65754243   8.88097015
 6.33504932   1.82877122   8.88097015
 7.91881165   0.91438561   8.88097015
 7.91881165  -0.91438561   8.88097015
 9.50257398  -1.82877122   8.88097015
 9.50257398  -3.65754243   8.88097015
11.08633632  -4.57192804   8.88097015
11.08633632  -6.40069926   8.88097015
 6.33504932   9.14385608   8.88097015
 6.33504932   7.31508486   8.88097015
 7.91881165   6.40069926   8.88097015
 7.91881165   4.57192804   8.88097015
 9.50257398   3.65754243   8.88097015
 9.50257398   1.82877122   8.88097015
11.08633632   0.91438561   8.88097015
11.08633632  -0.91438561   8.88097015
12.67009865  -1.82877122   8.88097015
12.67009865  -3.65754243   8.88097015
 7.91881165  11.88701290   8.88097015
 7.91881165  10.05824169   8.88097015
 9.50257398   9.14385608   8.88097015
 9.50257398   7.31508486   8.88097015
11.08633632   6.40069926   8.88097015
11.08633632   4.57192804   8.88097015
12.67009865   3.65754243   8.88097015
12.67009865   1.82877122   8.88097015
14.25386098   0.91438561   8.88097015
14.25386098  -0.91438561   8.88097015
 1.58376233   0.91438561  12.43335821
 1.58376233  -0.91438561  12.43335821
 3.16752466  -1.82877122  12.43335821
 3.16752466  -3.65754243  12.43335821
 4.75128699  -4.57192804  12.43335821
 4.75128699  -6.40069926  12.43335821
 6.33504932  -7.31508486  12.43335821
 6.33504932  -9.14385608  12.43335821
 7.91881165 -10.05824169  12.43335821
 7.91881165 -11.88701290  12.43335821
 3.16752466   3.65754243  12.43335821
```

```
 3.16752466   1.82877122  12.43335821
 4.75128699   0.91438561  12.43335821
 4.75128699  -0.91438561  12.43335821
 6.33504932  -1.82877122  12.43335821
 6.33504932  -3.65754243  12.43335821
 7.91881165  -4.57192804  12.43335821
 7.91881165  -6.40069926  12.43335821
 9.50257398  -7.31508486  12.43335821
 9.50257398  -9.14385608  12.43335821
 4.75128699   6.40069926  12.43335821
 4.75128699   4.57192804  12.43335821
 6.33504932   3.65754243  12.43335821
 6.33504932   1.82877122  12.43335821
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
 9.50257398   1.82877122  12.43335821
11.08633632   0.91438561  12.43335821
11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
12.67009865  -3.65754243  12.43335821
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
 4.75128699  -4.57192804  15.98574627
 4.75128699  -6.40069926  15.98574627
 6.33504932  -7.31508486  15.98574627
 6.33504932  -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466   3.65754243  15.98574627
 3.16752466   1.82877122  15.98574627
 4.75128699   0.91438561  15.98574627
 4.75128699  -0.91438561  15.98574627
 6.33504932  -1.82877122  15.98574627
 6.33504932  -3.65754243  15.98574627
 7.91881165  -4.57192804  15.98574627
 7.91881165  -6.40069926  15.98574627
 9.50257398  -7.31508486  15.98574627
 9.50257398  -9.14385608  15.98574627
 4.75128699   6.40069926  15.98574627
 4.75128699   4.57192804  15.98574627
 6.33504932   3.65754243  15.98574627
```

```
      6.33504932         1.82877122        15.98574627
      7.91881165         0.91438561        15.98574627
      7.91881165        -0.91438561        15.98574627
      9.50257398        -1.82877122        15.98574627
      9.50257398        -3.65754243        15.98574627
     11.08633632        -4.57192804        15.98574627
     11.08633632        -6.40069926        15.98574627
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
```

Listing 14: Structural input file for configuration: 5x5x5 B inter.

5x5x5_Cu_B POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr  B  Cu
   125     249     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
      4.75128699         8.22947047         0.00000000
      6.33504932         5.48631365         0.00000000
      7.91881165         2.74315682         0.00000000
      9.50257398         0.00000000         0.00000000
     11.08633632        -2.74315682         0.00000000
      6.33504932        10.97262730         0.00000000
```

```
 7.91881165   8.22947047   0.00000000
 9.50257398   5.48631365   0.00000000
11.08633632   2.74315682   0.00000000
12.67009865   0.00000000   0.00000000
 0.00000000   0.00000000   3.55238806
 1.58376233  -2.74315682   3.55238806
 3.16752466  -5.48631365   3.55238806
 4.75128699  -8.22947047   3.55238806
 6.33504932 -10.97262730   3.55238806
 1.58376233   2.74315682   3.55238806
 3.16752466   0.00000000   3.55238806
 4.75128699  -2.74315682   3.55238806
 6.33504932  -5.48631365   3.55238806
 7.91881165  -8.22947047   3.55238806
 3.16752466   5.48631365   3.55238806
 4.75128699   2.74315682   3.55238806
 6.33504932   0.00000000   3.55238806
 7.91881165  -2.74315682   3.55238806
 9.50257398  -5.48631365   3.55238806
 4.75128699   8.22947047   3.55238806
 6.33504932   5.48631365   3.55238806
 7.91881165   2.74315682   3.55238806
 9.50257398   0.00000000   3.55238806
11.08633632  -2.74315682   3.55238806
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
```

```
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
```

```
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
11.08633632  -0.91438561   1.77619403
12.67009865  -1.82877122   1.77619403
12.67009865  -3.65754243   1.77619403
 7.91881165  11.88701290   1.77619403
 7.91881165  10.05824169   1.77619403
 9.50257398   9.14385608   1.77619403
 9.50257398   7.31508486   1.77619403
11.08633632   6.40069926   1.77619403
11.08633632   4.57192804   1.77619403
12.67009865   3.65754243   1.77619403
12.67009865   1.82877122   1.77619403
14.25386098   0.91438561   1.77619403
14.25386098  -0.91438561   1.77619403
 1.58376233   0.91438561   5.32858209
 1.58376233  -0.91438561   5.32858209
 3.16752466  -1.82877122   5.32858209
 3.16752466  -3.65754243   5.32858209
 4.75128699  -4.57192804   5.32858209
 4.75128699  -6.40069926   5.32858209
 6.33504932  -7.31508486   5.32858209
 6.33504932  -9.14385608   5.32858209
 7.91881165 -10.05824169   5.32858209
 7.91881165 -11.88701290   5.32858209
 3.16752466   3.65754243   5.32858209
 3.16752466   1.82877122   5.32858209
 4.75128699   0.91438561   5.32858209
 4.75128699  -0.91438561   5.32858209
 6.33504932  -1.82877122   5.32858209
 6.33504932  -3.65754243   5.32858209
 7.91881165  -4.57192804   5.32858209
 7.91881165  -6.40069926   5.32858209
 9.50257398  -7.31508486   5.32858209
 9.50257398  -9.14385608   5.32858209
 4.75128699   6.40069926   5.32858209
 4.75128699   4.57192804   5.32858209
 6.33504932   3.65754243   5.32858209
 6.33504932   1.82877122   5.32858209
 7.91881165   0.91438561   5.32858209
 7.91881165  -0.91438561   5.32858209
 9.50257398  -1.82877122   5.32858209
 9.50257398  -3.65754243   5.32858209
11.08633632  -4.57192804   5.32858209
11.08633632  -6.40069926   5.32858209
 6.33504932   9.14385608   5.32858209
 6.33504932   7.31508486   5.32858209
```

```
 7.91881165  6.40069926  5.32858209
 7.91881165  4.57192804  5.32858209
 9.50257398  3.65754243  5.32858209
 9.50257398  1.82877122  5.32858209
11.08633632  0.91438561  5.32858209
11.08633632 -0.91438561  5.32858209
12.67009865 -1.82877122  5.32858209
12.67009865 -3.65754243  5.32858209
 7.91881165 11.88701290  5.32858209
 7.91881165 10.05824169  5.32858209
 9.50257398  9.14385608  5.32858209
 9.50257398  7.31508486  5.32858209
11.08633632  6.40069926  5.32858209
11.08633632  4.57192804  5.32858209
12.67009865  3.65754243  5.32858209
12.67009865  1.82877122  5.32858209
14.25386098  0.91438561  5.32858209
14.25386098 -0.91438561  5.32858209
 1.58376233  0.91438561  8.88097015
 1.58376233 -0.91438561  8.88097015
 3.16752466 -1.82877122  8.88097015
 3.16752466 -3.65754243  8.88097015
 4.75128699 -4.57192804  8.88097015
 4.75128699 -6.40069926  8.88097015
 6.33504932 -7.31508486  8.88097015
 6.33504932 -9.14385608  8.88097015
 7.91881165 -10.05824169  8.88097015
 7.91881165 -11.88701290  8.88097015
 3.16752466  3.65754243  8.88097015
 3.16752466  1.82877122  8.88097015
 4.75128699  0.91438561  8.88097015
 4.75128699 -0.91438561  8.88097015
 6.33504932 -1.82877122  8.88097015
 6.33504932 -3.65754243  8.88097015
 7.91881165 -4.57192804  8.88097015
 7.91881165 -6.40069926  8.88097015
 9.50257398 -7.31508486  8.88097015
 9.50257398 -9.14385608  8.88097015
 4.75128699  6.40069926  8.88097015
 4.75128699  4.57192804  8.88097015
 6.33504932  3.65754243  8.88097015
 6.33504932  1.82877122  8.88097015
 7.91881165  0.91438561  8.88097015
 7.91881165 -0.91438561  8.88097015
 9.50257398 -1.82877122  8.88097015
 9.50257398 -3.65754243  8.88097015
11.08633632 -4.57192804  8.88097015
11.08633632 -6.40069926  8.88097015
 6.33504932  9.14385608  8.88097015
 6.33504932  7.31508486  8.88097015
 7.91881165  6.40069926  8.88097015
 7.91881165  4.57192804  8.88097015
 9.50257398  3.65754243  8.88097015
 9.50257398  1.82877122  8.88097015
11.08633632  0.91438561  8.88097015
11.08633632 -0.91438561  8.88097015
12.67009865 -1.82877122  8.88097015
12.67009865 -3.65754243  8.88097015
 7.91881165 11.88701290  8.88097015
 7.91881165 10.05824169  8.88097015
 9.50257398  9.14385608  8.88097015
 9.50257398  7.31508486  8.88097015
```

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 11.08633632   6.40069926   8.88097015
 11.08633632   4.57192804   8.88097015
 12.67009865   3.65754243   8.88097015
 12.67009865   1.82877122   8.88097015
 14.25386098   0.91438561   8.88097015
 14.25386098  -0.91438561   8.88097015
  1.58376233   0.91438561  12.43335821
  1.58376233  -0.91438561  12.43335821
  3.16752466  -1.82877122  12.43335821
  3.16752466  -3.65754243  12.43335821
  4.75128699  -4.57192804  12.43335821
  4.75128699  -6.40069926  12.43335821
  6.33504932  -7.31508486  12.43335821
  6.33504932  -9.14385608  12.43335821
  7.91881165 -10.05824169  12.43335821
  7.91881165 -11.88701290  12.43335821
  3.16752466   3.65754243  12.43335821
  3.16752466   1.82877122  12.43335821
  4.75128699   0.91438561  12.43335821
  4.75128699  -0.91438561  12.43335821
  6.33504932  -1.82877122  12.43335821
  6.33504932  -3.65754243  12.43335821
  7.91881165  -4.57192804  12.43335821
  7.91881165  -6.40069926  12.43335821
  9.50257398  -7.31508486  12.43335821
  9.50257398  -9.14385608  12.43335821
  4.75128699   6.40069926  12.43335821
  4.75128699   4.57192804  12.43335821
  6.33504932   3.65754243  12.43335821
  6.33504932   1.82877122  12.43335821
  7.91881165   0.91438561  12.43335821
  7.91881165  -0.91438561  12.43335821
  9.50257398  -1.82877122  12.43335821
  9.50257398  -3.65754243  12.43335821
 11.08633632  -4.57192804  12.43335821
 11.08633632  -6.40069926  12.43335821
  6.33504932   9.14385608  12.43335821
  6.33504932   7.31508486  12.43335821
  7.91881165   6.40069926  12.43335821
  7.91881165   4.57192804  12.43335821
  9.50257398   3.65754243  12.43335821
  9.50257398   1.82877122  12.43335821
 11.08633632   0.91438561  12.43335821
 11.08633632  -0.91438561  12.43335821
 12.67009865  -1.82877122  12.43335821
 12.67009865  -3.65754243  12.43335821
  7.91881165  11.88701290  12.43335821
  7.91881165  10.05824169  12.43335821
  9.50257398   9.14385608  12.43335821
  9.50257398   7.31508486  12.43335821
 11.08633632   6.40069926  12.43335821
 11.08633632   4.57192804  12.43335821
 12.67009865   3.65754243  12.43335821
 12.67009865   1.82877122  12.43335821
 14.25386098   0.91438561  12.43335821
 14.25386098  -0.91438561  12.43335821
  1.58376233   0.91438561  15.98574627
  1.58376233  -0.91438561  15.98574627
  3.16752466  -1.82877122  15.98574627
  3.16752466  -3.65754243  15.98574627
  4.75128699  -4.57192804  15.98574627
  4.75128699  -6.40069926  15.98574627
```

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      6.33504932        -7.31508486        15.98574627
      6.33504932        -9.14385608        15.98574627
      7.91881165       -10.05824169        15.98574627
      7.91881165       -11.88701290        15.98574627
      3.16752466         3.65754243        15.98574627
      3.16752466         1.82877122        15.98574627
      4.75128699         0.91438561        15.98574627
      4.75128699        -0.91438561        15.98574627
      6.33504932        -1.82877122        15.98574627
      6.33504932        -3.65754243        15.98574627
      7.91881165        -4.57192804        15.98574627
      7.91881165        -6.40069926        15.98574627
      9.50257398        -7.31508486        15.98574627
      9.50257398        -9.14385608        15.98574627
      4.75128699         6.40069926        15.98574627
      4.75128699         4.57192804        15.98574627
      6.33504932         3.65754243        15.98574627
      6.33504932         1.82877122        15.98574627
      7.91881165         0.91438561        15.98574627
      7.91881165        -0.91438561        15.98574627
      9.50257398        -1.82877122        15.98574627
      9.50257398        -3.65754243        15.98574627
     11.08633632        -4.57192804        15.98574627
     11.08633632        -6.40069926        15.98574627
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
```

Listing 15: Structural input file for configuration: 5x5x5 Cu B.

5x5x5_Cu_Zr POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr   B   Cu
   145     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
```

```
 6.33504932      -10.97262730        0.00000000
 1.58376233        2.74315682        0.00000000
 3.16752466        0.00000000        0.00000000
 4.75128699       -2.74315682        0.00000000
 6.33504932       -5.48631365        0.00000000
 7.91881165       -8.22947047        0.00000000
 3.16752466        5.48631365        0.00000000
 4.75128699        2.74315682        0.00000000
 6.33504932        0.00000000        0.00000000
 7.91881165       -2.74315682        0.00000000
 9.50257398       -5.48631365        0.00000000
 4.75128699        8.22947047        0.00000000
 6.33504932        5.48631365        0.00000000
 7.91881165        2.74315682        0.00000000
 9.50257398        0.00000000        0.00000000
11.08633632       -2.74315682        0.00000000
 6.33504932       10.97262730        0.00000000
 7.91881165        8.22947047        0.00000000
 9.50257398        5.48631365        0.00000000
11.08633632        2.74315682        0.00000000
12.67009865        0.00000000        0.00000000
 0.00000000        0.00000000        3.55238806
 1.58376233       -2.74315682        3.55238806
 3.16752466       -5.48631365        3.55238806
 4.75128699       -8.22947047        3.55238806
 6.33504932      -10.97262730        3.55238806
 1.58376233        2.74315682        3.55238806
 3.16752466        0.00000000        3.55238806
 4.75128699       -2.74315682        3.55238806
 6.33504932       -5.48631365        3.55238806
 7.91881165       -8.22947047        3.55238806
 3.16752466        5.48631365        3.55238806
 4.75128699        2.74315682        3.55238806
 6.33504932        0.00000000        3.55238806
 7.91881165       -2.74315682        3.55238806
 9.50257398       -5.48631365        3.55238806
 4.75128699        8.22947047        3.55238806
 6.33504932        5.48631365        3.55238806
 7.91881165        2.74315682        3.55238806
 9.50257398        0.00000000        3.55238806
11.08633632       -2.74315682        3.55238806
 6.33504932       10.97262730        3.55238806
 7.91881165        8.22947047        3.55238806
 9.50257398        5.48631365        3.55238806
11.08633632        2.74315682        3.55238806
12.67009865        0.00000000        3.55238806
 0.00000000        0.00000000        7.10477612
 1.58376233       -2.74315682        7.10477612
 3.16752466       -5.48631365        7.10477612
 4.75128699       -8.22947047        7.10477612
 6.33504932      -10.97262730        7.10477612
 3.16752466        0.00000000        7.10477612
 4.75128699       -2.74315682        7.10477612
 6.33504932       -5.48631365        7.10477612
 7.91881165       -8.22947047        7.10477612
 3.16752466        5.48631365        7.10477612
 4.75128699        2.74315682        7.10477612
 6.33504932        0.00000000        7.10477612
 7.91881165       -2.74315682        7.10477612
 9.50257398       -5.48631365        7.10477612
 4.75128699        8.22947047        7.10477612
 6.33504932        5.48631365        7.10477612
```

```
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
```

```
 4.75128699  -4.57192804  1.77619403
 4.75128699  -6.40069926  1.77619403
 6.33504932  -7.31508486  1.77619403
 6.33504932  -9.14385608  1.77619403
 7.91881165 -10.05824169  1.77619403
 7.91881165 -11.88701290  1.77619403
 3.16752466   3.65754243  1.77619403
 3.16752466   1.82877122  1.77619403
 4.75128699   0.91438561  1.77619403
 4.75128699  -0.91438561  1.77619403
 6.33504932  -1.82877122  1.77619403
 6.33504932  -3.65754243  1.77619403
 7.91881165  -4.57192804  1.77619403
 7.91881165  -6.40069926  1.77619403
 9.50257398  -7.31508486  1.77619403
 9.50257398  -9.14385608  1.77619403
 4.75128699   6.40069926  1.77619403
 4.75128699   4.57192804  1.77619403
 6.33504932   3.65754243  1.77619403
 6.33504932   1.82877122  1.77619403
 7.91881165   0.91438561  1.77619403
 7.91881165  -0.91438561  1.77619403
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 9.50257398  -3.65754243  1.77619403
11.08633632  -4.57192804  1.77619403
11.08633632  -6.40069926  1.77619403
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 6.33504932   7.31508486  1.77619403
 7.91881165   6.40069926  1.77619403
 7.91881165   4.57192804  1.77619403
 9.50257398   3.65754243  1.77619403
 9.50257398   1.82877122  1.77619403
11.08633632   0.91438561  1.77619403
11.08633632  -0.91438561  1.77619403
12.67009865  -1.82877122  1.77619403
12.67009865  -3.65754243  1.77619403
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 9.50257398   9.14385608  1.77619403
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11.08633632   6.40069926  1.77619403
11.08633632   4.57192804  1.77619403
12.67009865   3.65754243  1.77619403
12.67009865   1.82877122  1.77619403
14.25386098   0.91438561  1.77619403
14.25386098  -0.91438561  1.77619403
 1.58376233   0.91438561  5.32858209
 1.58376233  -0.91438561  5.32858209
 3.16752466  -1.82877122  5.32858209
 3.16752466  -3.65754243  5.32858209
 4.75128699  -4.57192804  5.32858209
 4.75128699  -6.40069926  5.32858209
 6.33504932  -7.31508486  5.32858209
 6.33504932  -9.14385608  5.32858209
 7.91881165 -10.05824169  5.32858209
 7.91881165 -11.88701290  5.32858209
 3.16752466   3.65754243  5.32858209
 3.16752466   1.82877122  5.32858209
 4.75128699   0.91438561  5.32858209
 4.75128699  -0.91438561  5.32858209
 6.33504932  -1.82877122  5.32858209
 6.33504932  -3.65754243  5.32858209
```

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 7.91881165  -6.40069926  5.32858209
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 9.50257398  -9.14385608  5.32858209
 4.75128699   6.40069926  5.32858209
 4.75128699   4.57192804  5.32858209
 6.33504932   3.65754243  5.32858209
 6.33504932   1.82877122  5.32858209
 7.91881165   0.91438561  5.32858209
 7.91881165  -0.91438561  5.32858209
 9.50257398  -1.82877122  5.32858209
 9.50257398  -3.65754243  5.32858209
11.08633632  -4.57192804  5.32858209
11.08633632  -6.40069926  5.32858209
 6.33504932   9.14385608  5.32858209
 6.33504932   7.31508486  5.32858209
 7.91881165   6.40069926  5.32858209
 7.91881165   4.57192804  5.32858209
 9.50257398   3.65754243  5.32858209
 9.50257398   1.82877122  5.32858209
11.08633632   0.91438561  5.32858209
11.08633632  -0.91438561  5.32858209
12.67009865  -1.82877122  5.32858209
12.67009865  -3.65754243  5.32858209
 7.91881165  11.88701290  5.32858209
 7.91881165  10.05824169  5.32858209
 9.50257398   9.14385608  5.32858209
 9.50257398   7.31508486  5.32858209
11.08633632   6.40069926  5.32858209
11.08633632   4.57192804  5.32858209
12.67009865   3.65754243  5.32858209
12.67009865   1.82877122  5.32858209
14.25386098   0.91438561  5.32858209
14.25386098  -0.91438561  5.32858209
 1.58376233   0.91438561  8.88097015
 1.58376233  -0.91438561  8.88097015
 3.16752466  -1.82877122  8.88097015
 3.16752466  -3.65754243  8.88097015
 4.75128699  -4.57192804  8.88097015
 4.75128699  -6.40069926  8.88097015
 6.33504932  -7.31508486  8.88097015
 6.33504932  -9.14385608  8.88097015
 7.91881165 -10.05824169  8.88097015
 7.91881165 -11.88701290  8.88097015
 3.16752466   3.65754243  8.88097015
 3.16752466   1.82877122  8.88097015
 4.75128699   0.91438561  8.88097015
 4.75128699  -0.91438561  8.88097015
 6.33504932  -1.82877122  8.88097015
 6.33504932  -3.65754243  8.88097015
 7.91881165  -4.57192804  8.88097015
 7.91881165  -6.40069926  8.88097015
 9.50257398  -7.31508486  8.88097015
 9.50257398  -9.14385608  8.88097015
 4.75128699   6.40069926  8.88097015
 4.75128699   4.57192804  8.88097015
 6.33504932   3.65754243  8.88097015
 6.33504932   1.82877122  8.88097015
 7.91881165   0.91438561  8.88097015
 7.91881165  -0.91438561  8.88097015
 9.50257398  -1.82877122  8.88097015
 9.50257398  -3.65754243  8.88097015
```

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 11.08633632   -6.40069926    8.88097015
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  6.33504932    7.31508486    8.88097015
  7.91881165    6.40069926    8.88097015
  7.91881165    4.57192804    8.88097015
  9.50257398    3.65754243    8.88097015
  9.50257398    1.82877122    8.88097015
 11.08633632    0.91438561    8.88097015
 11.08633632   -0.91438561    8.88097015
 12.67009865   -1.82877122    8.88097015
 12.67009865   -3.65754243    8.88097015
  7.91881165   11.88701290    8.88097015
  7.91881165   10.05824169    8.88097015
  9.50257398    9.14385608    8.88097015
  9.50257398    7.31508486    8.88097015
 11.08633632    6.40069926    8.88097015
 11.08633632    4.57192804    8.88097015
 12.67009865    3.65754243    8.88097015
 12.67009865    1.82877122    8.88097015
 14.25386098    0.91438561    8.88097015
 14.25386098   -0.91438561    8.88097015
  1.58376233    0.91438561   12.43335821
  1.58376233   -0.91438561   12.43335821
  3.16752466   -1.82877122   12.43335821
  3.16752466   -3.65754243   12.43335821
  4.75128699   -4.57192804   12.43335821
  4.75128699   -6.40069926   12.43335821
  6.33504932   -7.31508486   12.43335821
  6.33504932   -9.14385608   12.43335821
  7.91881165  -10.05824169   12.43335821
  7.91881165  -11.88701290   12.43335821
  3.16752466    3.65754243   12.43335821
  3.16752466    1.82877122   12.43335821
  4.75128699    0.91438561   12.43335821
  4.75128699   -0.91438561   12.43335821
  6.33504932   -1.82877122   12.43335821
  6.33504932   -3.65754243   12.43335821
  7.91881165   -4.57192804   12.43335821
  7.91881165   -6.40069926   12.43335821
  9.50257398   -7.31508486   12.43335821
  9.50257398   -9.14385608   12.43335821
  4.75128699    6.40069926   12.43335821
  4.75128699    4.57192804   12.43335821
  6.33504932    3.65754243   12.43335821
  6.33504932    1.82877122   12.43335821
  7.91881165    0.91438561   12.43335821
  7.91881165   -0.91438561   12.43335821
  9.50257398   -1.82877122   12.43335821
  9.50257398   -3.65754243   12.43335821
 11.08633632   -4.57192804   12.43335821
 11.08633632   -6.40069926   12.43335821
  6.33504932    9.14385608   12.43335821
  6.33504932    7.31508486   12.43335821
  7.91881165    6.40069926   12.43335821
  7.91881165    4.57192804   12.43335821
  9.50257398    3.65754243   12.43335821
  9.50257398    1.82877122   12.43335821
 11.08633632    0.91438561   12.43335821
 11.08633632   -0.91438561   12.43335821
 12.67009865   -1.82877122   12.43335821
 12.67009865   -3.65754243   12.43335821
```

```
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
 4.75128699  -4.57192804  15.98574627
 4.75128699  -6.40069926  15.98574627
 6.33504932  -7.31508486  15.98574627
 6.33504932  -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466   3.65754243  15.98574627
 3.16752466   1.82877122  15.98574627
 4.75128699   0.91438561  15.98574627
 4.75128699  -0.91438561  15.98574627
 6.33504932  -1.82877122  15.98574627
 6.33504932  -3.65754243  15.98574627
 7.91881165  -4.57192804  15.98574627
 7.91881165  -6.40069926  15.98574627
 9.50257398  -7.31508486  15.98574627
 9.50257398  -9.14385608  15.98574627
 4.75128699   6.40069926  15.98574627
 4.75128699   4.57192804  15.98574627
 6.33504932   3.65754243  15.98574627
 6.33504932   1.82877122  15.98574627
 7.91881165   0.91438561  15.98574627
 7.91881165  -0.91438561  15.98574627
 9.50257398  -1.82877122  15.98574627
 9.50257398  -3.65754243  15.98574627
11.08633632  -4.57192804  15.98574627
11.08633632  -6.40069926  15.98574627
 6.33504932   9.14385608  15.98574627
 6.33504932   7.31508486  15.98574627
 7.91881165   6.40069926  15.98574627
 7.91881165   4.57192804  15.98574627
 9.50257398   3.65754243  15.98574627
 9.50257398   1.82877122  15.98574627
11.08633632   0.91438561  15.98574627
11.08633632  -0.91438561  15.98574627
12.67009865  -1.82877122  15.98574627
12.67009865  -3.65754243  15.98574627
 7.91881165  11.88701290  15.98574627
 7.91881165  10.05824169  15.98574627
 9.50257398   9.14385608  15.98574627
 9.50257398   7.31508486  15.98574627
11.08633632   6.40069926  15.98574627
11.08633632   4.57192804  15.98574627
12.67009865   3.65754243  15.98574627
12.67009865   1.82877122  15.98574627
14.25386098   0.91438561  15.98574627
14.25386098  -0.91438561  15.98574627
 1.58376233   2.74315682   7.10477612
```

Listing 16: Structural input file for configuration: 5x5x5 Cu Zr.

5x5x5_H_B_bridge POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr   B   H
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
      4.75128699         8.22947047         0.00000000
      6.33504932         5.48631365         0.00000000
      7.91881165         2.74315682         0.00000000
      9.50257398         0.00000000         0.00000000
     11.08633632        -2.74315682         0.00000000
      6.33504932        10.97262730         0.00000000
      7.91881165         8.22947047         0.00000000
      9.50257398         5.48631365         0.00000000
     11.08633632         2.74315682         0.00000000
     12.67009865         0.00000000         0.00000000
      0.00000000         0.00000000         3.55238806
      1.58376233        -2.74315682         3.55238806
      3.16752466        -5.48631365         3.55238806
      4.75128699        -8.22947047         3.55238806
      6.33504932       -10.97262730         3.55238806
      1.58376233         2.74315682         3.55238806
      3.16752466         0.00000000         3.55238806
      4.75128699        -2.74315682         3.55238806
      6.33504932        -5.48631365         3.55238806
      7.91881165        -8.22947047         3.55238806
      3.16752466         5.48631365         3.55238806
      4.75128699         2.74315682         3.55238806
      6.33504932         0.00000000         3.55238806
      7.91881165        -2.74315682         3.55238806
      9.50257398        -5.48631365         3.55238806
      4.75128699         8.22947047         3.55238806
      6.33504932         5.48631365         3.55238806
      7.91881165         2.74315682         3.55238806
      9.50257398         0.00000000         3.55238806
     11.08633632        -2.74315682         3.55238806
      6.33504932        10.97262730         3.55238806
      7.91881165         8.22947047         3.55238806
```

```
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
```

```
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
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 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
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 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
11.08633632  -0.91438561   1.77619403
12.67009865  -1.82877122   1.77619403
12.67009865  -3.65754243   1.77619403
 7.91881165  11.88701290   1.77619403
 7.91881165  10.05824169   1.77619403
 9.50257398   9.14385608   1.77619403
 9.50257398   7.31508486   1.77619403
11.08633632   6.40069926   1.77619403
11.08633632   4.57192804   1.77619403
```

```
 12.67009865   3.65754243   1.77619403
 12.67009865   1.82877122   1.77619403
 14.25386098   0.91438561   1.77619403
 14.25386098  -0.91438561   1.77619403
  1.58376233   0.91438561   5.32858209
  1.58376233  -0.91438561   5.32858209
  3.16752466  -1.82877122   5.32858209
  3.16752466  -3.65754243   5.32858209
  4.75128699  -4.57192804   5.32858209
  4.75128699  -6.40069926   5.32858209
  6.33504932  -7.31508486   5.32858209
  6.33504932  -9.14385608   5.32858209
  7.91881165 -10.05824169   5.32858209
  7.91881165 -11.88701290   5.32858209
  3.16752466   3.65754243   5.32858209
  3.16752466   1.82877122   5.32858209
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  4.75128699  -0.91438561   5.32858209
  6.33504932  -1.82877122   5.32858209
  6.33504932  -3.65754243   5.32858209
  7.91881165  -4.57192804   5.32858209
  7.91881165  -6.40069926   5.32858209
  9.50257398  -7.31508486   5.32858209
  9.50257398  -9.14385608   5.32858209
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  4.75128699   4.57192804   5.32858209
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  6.33504932   1.82877122   5.32858209
  7.91881165   0.91438561   5.32858209
  7.91881165  -0.91438561   5.32858209
  9.50257398  -1.82877122   5.32858209
  9.50257398  -3.65754243   5.32858209
 11.08633632  -4.57192804   5.32858209
 11.08633632  -6.40069926   5.32858209
  6.33504932   9.14385608   5.32858209
  6.33504932   7.31508486   5.32858209
  7.91881165   6.40069926   5.32858209
  7.91881165   4.57192804   5.32858209
  9.50257398   3.65754243   5.32858209
  9.50257398   1.82877122   5.32858209
 11.08633632   0.91438561   5.32858209
 11.08633632  -0.91438561   5.32858209
 12.67009865  -1.82877122   5.32858209
 12.67009865  -3.65754243   5.32858209
  7.91881165  11.88701290   5.32858209
  7.91881165  10.05824169   5.32858209
  9.50257398   9.14385608   5.32858209
  9.50257398   7.31508486   5.32858209
 11.08633632   6.40069926   5.32858209
 11.08633632   4.57192804   5.32858209
 12.67009865   3.65754243   5.32858209
 12.67009865   1.82877122   5.32858209
 14.25386098   0.91438561   5.32858209
 14.25386098  -0.91438561   5.32858209
  1.58376233   0.91438561   8.88097015
  1.58376233  -0.91438561   8.88097015
  3.16752466  -1.82877122   8.88097015
  3.16752466  -3.65754243   8.88097015
  4.75128699  -4.57192804   8.88097015
  4.75128699  -6.40069926   8.88097015
  6.33504932  -7.31508486   8.88097015
  6.33504932  -9.14385608   8.88097015
```

```
 7.91881165  -10.05824169   8.88097015
 7.91881165  -11.88701290   8.88097015
 3.16752466    3.65754243   8.88097015
 3.16752466    1.82877122   8.88097015
 4.75128699    0.91438561   8.88097015
 4.75128699   -0.91438561   8.88097015
 6.33504932   -1.82877122   8.88097015
 6.33504932   -3.65754243   8.88097015
 7.91881165   -4.57192804   8.88097015
 7.91881165   -6.40069926   8.88097015
 9.50257398   -7.31508486   8.88097015
 9.50257398   -9.14385608   8.88097015
 4.75128699    6.40069926   8.88097015
 4.75128699    4.57192804   8.88097015
 6.33504932    3.65754243   8.88097015
 6.33504932    1.82877122   8.88097015
 7.91881165    0.91438561   8.88097015
 7.91881165   -0.91438561   8.88097015
 9.50257398   -1.82877122   8.88097015
 9.50257398   -3.65754243   8.88097015
11.08633632   -4.57192804   8.88097015
11.08633632   -6.40069926   8.88097015
 6.33504932    9.14385608   8.88097015
 6.33504932    7.31508486   8.88097015
 7.91881165    6.40069926   8.88097015
 7.91881165    4.57192804   8.88097015
 9.50257398    3.65754243   8.88097015
 9.50257398    1.82877122   8.88097015
11.08633632    0.91438561   8.88097015
11.08633632   -0.91438561   8.88097015
12.67009865   -1.82877122   8.88097015
12.67009865   -3.65754243   8.88097015
 7.91881165   11.88701290   8.88097015
 7.91881165   10.05824169   8.88097015
 9.50257398    9.14385608   8.88097015
 9.50257398    7.31508486   8.88097015
11.08633632    6.40069926   8.88097015
11.08633632    4.57192804   8.88097015
12.67009865    3.65754243   8.88097015
12.67009865    1.82877122   8.88097015
14.25386098    0.91438561   8.88097015
14.25386098   -0.91438561   8.88097015
 1.58376233    0.91438561  12.43335821
 1.58376233   -0.91438561  12.43335821
 3.16752466   -1.82877122  12.43335821
 3.16752466   -3.65754243  12.43335821
 4.75128699   -4.57192804  12.43335821
 4.75128699   -6.40069926  12.43335821
 6.33504932   -7.31508486  12.43335821
 6.33504932   -9.14385608  12.43335821
 7.91881165  -10.05824169  12.43335821
 7.91881165  -11.88701290  12.43335821
 3.16752466    3.65754243  12.43335821
 3.16752466    1.82877122  12.43335821
 4.75128699    0.91438561  12.43335821
 4.75128699   -0.91438561  12.43335821
 6.33504932   -1.82877122  12.43335821
 6.33504932   -3.65754243  12.43335821
 7.91881165   -4.57192804  12.43335821
 7.91881165   -6.40069926  12.43335821
 9.50257398   -7.31508486  12.43335821
 9.50257398   -9.14385608  12.43335821
```

```
 4.75128699   6.40069926  12.43335821
 4.75128699   4.57192804  12.43335821
 6.33504932   3.65754243  12.43335821
 6.33504932   1.82877122  12.43335821
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
 9.50257398   1.82877122  12.43335821
11.08633632   0.91438561  12.43335821
11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
12.67009865  -3.65754243  12.43335821
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
 4.75128699  -4.57192804  15.98574627
 4.75128699  -6.40069926  15.98574627
 6.33504932  -7.31508486  15.98574627
 6.33504932  -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466   3.65754243  15.98574627
 3.16752466   1.82877122  15.98574627
 4.75128699   0.91438561  15.98574627
 4.75128699  -0.91438561  15.98574627
 6.33504932  -1.82877122  15.98574627
 6.33504932  -3.65754243  15.98574627
 7.91881165  -4.57192804  15.98574627
 7.91881165  -6.40069926  15.98574627
 9.50257398  -7.31508486  15.98574627
 9.50257398  -9.14385608  15.98574627
 4.75128699   6.40069926  15.98574627
 4.75128699   4.57192804  15.98574627
 6.33504932   3.65754243  15.98574627
 6.33504932   1.82877122  15.98574627
 7.91881165   0.91438561  15.98574627
 7.91881165  -0.91438561  15.98574627
 9.50257398  -1.82877122  15.98574627
 9.50257398  -3.65754243  15.98574627
11.08633632  -4.57192804  15.98574627
11.08633632  -6.40069926  15.98574627
 6.33504932   9.14385608  15.98574627
 6.33504932   7.31508486  15.98574627
```

```
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   7.9   0.0  15.98575
```

Listing 17: Structural input file for configuration: 5x5x5 H B bridge.

5x5x5_H_B_ring POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr   B   H
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
      4.75128699         8.22947047         0.00000000
      6.33504932         5.48631365         0.00000000
      7.91881165         2.74315682         0.00000000
      9.50257398         0.00000000         0.00000000
     11.08633632        -2.74315682         0.00000000
      6.33504932        10.97262730         0.00000000
      7.91881165         8.22947047         0.00000000
      9.50257398         5.48631365         0.00000000
     11.08633632         2.74315682         0.00000000
     12.67009865         0.00000000         0.00000000
      0.00000000         0.00000000         3.55238806
      1.58376233        -2.74315682         3.55238806
      3.16752466        -5.48631365         3.55238806
      4.75128699        -8.22947047         3.55238806
```

```
 6.33504932      -10.97262730        3.55238806
 1.58376233        2.74315682        3.55238806
 3.16752466        0.00000000        3.55238806
 4.75128699       -2.74315682        3.55238806
 6.33504932       -5.48631365        3.55238806
 7.91881165       -8.22947047        3.55238806
 3.16752466        5.48631365        3.55238806
 4.75128699        2.74315682        3.55238806
 6.33504932        0.00000000        3.55238806
 7.91881165       -2.74315682        3.55238806
 9.50257398       -5.48631365        3.55238806
 4.75128699        8.22947047        3.55238806
 6.33504932        5.48631365        3.55238806
 7.91881165        2.74315682        3.55238806
 9.50257398        0.00000000        3.55238806
11.08633632       -2.74315682        3.55238806
 6.33504932       10.97262730        3.55238806
 7.91881165        8.22947047        3.55238806
 9.50257398        5.48631365        3.55238806
11.08633632        2.74315682        3.55238806
12.67009865        0.00000000        3.55238806
 0.00000000        0.00000000        7.10477612
 1.58376233       -2.74315682        7.10477612
 3.16752466       -5.48631365        7.10477612
 4.75128699       -8.22947047        7.10477612
 6.33504932      -10.97262730        7.10477612
 1.58376233        2.74315682        7.10477612
 3.16752466        0.00000000        7.10477612
 4.75128699       -2.74315682        7.10477612
 6.33504932       -5.48631365        7.10477612
 7.91881165       -8.22947047        7.10477612
 3.16752466        5.48631365        7.10477612
 4.75128699        2.74315682        7.10477612
 6.33504932        0.00000000        7.10477612
 7.91881165       -2.74315682        7.10477612
 9.50257398       -5.48631365        7.10477612
 4.75128699        8.22947047        7.10477612
 6.33504932        5.48631365        7.10477612
 7.91881165        2.74315682        7.10477612
 9.50257398        0.00000000        7.10477612
11.08633632       -2.74315682        7.10477612
 6.33504932       10.97262730        7.10477612
 7.91881165        8.22947047        7.10477612
 9.50257398        5.48631365        7.10477612
11.08633632        2.74315682        7.10477612
12.67009865        0.00000000        7.10477612
 0.00000000        0.00000000       10.65716418
 1.58376233       -2.74315682       10.65716418
 3.16752466       -5.48631365       10.65716418
 4.75128699       -8.22947047       10.65716418
 6.33504932      -10.97262730       10.65716418
 1.58376233        2.74315682       10.65716418
 3.16752466        0.00000000       10.65716418
 4.75128699       -2.74315682       10.65716418
 6.33504932       -5.48631365       10.65716418
 7.91881165       -8.22947047       10.65716418
 3.16752466        5.48631365       10.65716418
 4.75128699        2.74315682       10.65716418
 6.33504932        0.00000000       10.65716418
 7.91881165       -2.74315682       10.65716418
 9.50257398       -5.48631365       10.65716418
 4.75128699        8.22947047       10.65716418
```

```
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
```

```
 11.08633632   -4.57192804    1.77619403
 11.08633632   -6.40069926    1.77619403
  6.33504932    9.14385608    1.77619403
  6.33504932    7.31508486    1.77619403
  7.91881165    6.40069926    1.77619403
  7.91881165    4.57192804    1.77619403
  9.50257398    3.65754243    1.77619403
  9.50257398    1.82877122    1.77619403
 11.08633632    0.91438561    1.77619403
 11.08633632   -0.91438561    1.77619403
 12.67009865   -1.82877122    1.77619403
 12.67009865   -3.65754243    1.77619403
  7.91881165   11.88701290    1.77619403
  7.91881165   10.05824169    1.77619403
  9.50257398    9.14385608    1.77619403
  9.50257398    7.31508486    1.77619403
 11.08633632    6.40069926    1.77619403
 11.08633632    4.57192804    1.77619403
 12.67009865    3.65754243    1.77619403
 12.67009865    1.82877122    1.77619403
 14.25386098    0.91438561    1.77619403
 14.25386098   -0.91438561    1.77619403
  1.58376233    0.91438561    5.32858209
  1.58376233   -0.91438561    5.32858209
  3.16752466   -1.82877122    5.32858209
  3.16752466   -3.65754243    5.32858209
  4.75128699   -4.57192804    5.32858209
  4.75128699   -6.40069926    5.32858209
  6.33504932   -7.31508486    5.32858209
  6.33504932   -9.14385608    5.32858209
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  7.91881165  -11.88701290    5.32858209
  3.16752466    3.65754243    5.32858209
  3.16752466    1.82877122    5.32858209
  4.75128699    0.91438561    5.32858209
  4.75128699   -0.91438561    5.32858209
  6.33504932   -1.82877122    5.32858209
  6.33504932   -3.65754243    5.32858209
  7.91881165   -4.57192804    5.32858209
  7.91881165   -6.40069926    5.32858209
  9.50257398   -7.31508486    5.32858209
  9.50257398   -9.14385608    5.32858209
  4.75128699    6.40069926    5.32858209
  4.75128699    4.57192804    5.32858209
  6.33504932    3.65754243    5.32858209
  6.33504932    1.82877122    5.32858209
  7.91881165    0.91438561    5.32858209
  7.91881165   -0.91438561    5.32858209
  9.50257398   -1.82877122    5.32858209
  9.50257398   -3.65754243    5.32858209
 11.08633632   -4.57192804    5.32858209
 11.08633632   -6.40069926    5.32858209
  6.33504932    9.14385608    5.32858209
  6.33504932    7.31508486    5.32858209
  7.91881165    6.40069926    5.32858209
  7.91881165    4.57192804    5.32858209
  9.50257398    3.65754243    5.32858209
  9.50257398    1.82877122    5.32858209
 11.08633632    0.91438561    5.32858209
 11.08633632   -0.91438561    5.32858209
 12.67009865   -1.82877122    5.32858209
 12.67009865   -3.65754243    5.32858209
```

```
 7.91881165  11.88701290   5.32858209
 7.91881165  10.05824169   5.32858209
 9.50257398   9.14385608   5.32858209
 9.50257398   7.31508486   5.32858209
11.08633632   6.40069926   5.32858209
11.08633632   4.57192804   5.32858209
12.67009865   3.65754243   5.32858209
12.67009865   1.82877122   5.32858209
14.25386098   0.91438561   5.32858209
14.25386098  -0.91438561   5.32858209
 1.58376233   0.91438561   8.88097015
 1.58376233  -0.91438561   8.88097015
 3.16752466  -1.82877122   8.88097015
 3.16752466  -3.65754243   8.88097015
 4.75128699  -4.57192804   8.88097015
 4.75128699  -6.40069926   8.88097015
 6.33504932  -7.31508486   8.88097015
 6.33504932  -9.14385608   8.88097015
 7.91881165 -10.05824169   8.88097015
 7.91881165 -11.88701290   8.88097015
 3.16752466   3.65754243   8.88097015
 3.16752466   1.82877122   8.88097015
 4.75128699   0.91438561   8.88097015
 4.75128699  -0.91438561   8.88097015
 6.33504932  -1.82877122   8.88097015
 6.33504932  -3.65754243   8.88097015
 7.91881165  -4.57192804   8.88097015
 7.91881165  -6.40069926   8.88097015
 9.50257398  -7.31508486   8.88097015
 9.50257398  -9.14385608   8.88097015
 4.75128699   6.40069926   8.88097015
 4.75128699   4.57192804   8.88097015
 6.33504932   3.65754243   8.88097015
 6.33504932   1.82877122   8.88097015
 7.91881165   0.91438561   8.88097015
 7.91881165  -0.91438561   8.88097015
 9.50257398  -1.82877122   8.88097015
 9.50257398  -3.65754243   8.88097015
11.08633632  -4.57192804   8.88097015
11.08633632  -6.40069926   8.88097015
 6.33504932   9.14385608   8.88097015
 6.33504932   7.31508486   8.88097015
 7.91881165   6.40069926   8.88097015
 7.91881165   4.57192804   8.88097015
 9.50257398   3.65754243   8.88097015
 9.50257398   1.82877122   8.88097015
11.08633632   0.91438561   8.88097015
11.08633632  -0.91438561   8.88097015
12.67009865  -1.82877122   8.88097015
12.67009865  -3.65754243   8.88097015
 7.91881165  11.88701290   8.88097015
 7.91881165  10.05824169   8.88097015
 9.50257398   9.14385608   8.88097015
 9.50257398   7.31508486   8.88097015
11.08633632   6.40069926   8.88097015
11.08633632   4.57192804   8.88097015
12.67009865   3.65754243   8.88097015
12.67009865   1.82877122   8.88097015
14.25386098   0.91438561   8.88097015
14.25386098  -0.91438561   8.88097015
 1.58376233   0.91438561  12.43335821
 1.58376233  -0.91438561  12.43335821
```

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 3.16752466  -1.82877122  12.43335821
 3.16752466  -3.65754243  12.43335821
 4.75128699  -4.57192804  12.43335821
 4.75128699  -6.40069926  12.43335821
 6.33504932  -7.31508486  12.43335821
 6.33504932  -9.14385608  12.43335821
 7.91881165 -10.05824169  12.43335821
 7.91881165 -11.88701290  12.43335821
 3.16752466   3.65754243  12.43335821
 3.16752466   1.82877122  12.43335821
 4.75128699   0.91438561  12.43335821
 4.75128699  -0.91438561  12.43335821
 6.33504932  -1.82877122  12.43335821
 6.33504932  -3.65754243  12.43335821
 7.91881165  -4.57192804  12.43335821
 7.91881165  -6.40069926  12.43335821
 9.50257398  -7.31508486  12.43335821
 9.50257398  -9.14385608  12.43335821
 4.75128699   6.40069926  12.43335821
 4.75128699   4.57192804  12.43335821
 6.33504932   3.65754243  12.43335821
 6.33504932   1.82877122  12.43335821
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
 9.50257398   1.82877122  12.43335821
11.08633632   0.91438561  12.43335821
11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
12.67009865  -3.65754243  12.43335821
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
 4.75128699  -4.57192804  15.98574627
 4.75128699  -6.40069926  15.98574627
 6.33504932  -7.31508486  15.98574627
 6.33504932  -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466   3.65754243  15.98574627
 3.16752466   1.82877122  15.98574627
 4.75128699   0.91438561  15.98574627
 4.75128699  -0.91438561  15.98574627
```

```
      6.33504932        -1.82877122        15.98574627
      6.33504932        -3.65754243        15.98574627
      7.91881165        -4.57192804        15.98574627
      7.91881165        -6.40069926        15.98574627
      9.50257398        -7.31508486        15.98574627
      9.50257398        -9.14385608        15.98574627
      4.75128699         6.40069926        15.98574627
      4.75128699         4.57192804        15.98574627
      6.33504932         3.65754243        15.98574627
      6.33504932         1.82877122        15.98574627
      7.91881165         0.91438561        15.98574627
      7.91881165        -0.91438561        15.98574627
      9.50257398        -1.82877122        15.98574627
      9.50257398        -3.65754243        15.98574627
     11.08633632        -4.57192804        15.98574627
     11.08633632        -6.40069926        15.98574627
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   6.33505  0  15.98575
```

Listing 18: Structural input file for configuration: 5x5x5 H B ring.

5x5x5_H_B_top POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr  B  H
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
```

```
 4.75128699   2.74315682   0.00000000
 6.33504932   0.00000000   0.00000000
 7.91881165  -2.74315682   0.00000000
 9.50257398  -5.48631365   0.00000000
 4.75128699   8.22947047   0.00000000
 6.33504932   5.48631365   0.00000000
 7.91881165   2.74315682   0.00000000
 9.50257398   0.00000000   0.00000000
11.08633632  -2.74315682   0.00000000
 6.33504932  10.97262730   0.00000000
 7.91881165   8.22947047   0.00000000
 9.50257398   5.48631365   0.00000000
11.08633632   2.74315682   0.00000000
12.67009865   0.00000000   0.00000000
 0.00000000   0.00000000   3.55238806
 1.58376233  -2.74315682   3.55238806
 3.16752466  -5.48631365   3.55238806
 4.75128699  -8.22947047   3.55238806
 6.33504932 -10.97262730   3.55238806
 1.58376233   2.74315682   3.55238806
 3.16752466   0.00000000   3.55238806
 4.75128699  -2.74315682   3.55238806
 6.33504932  -5.48631365   3.55238806
 7.91881165  -8.22947047   3.55238806
 3.16752466   5.48631365   3.55238806
 4.75128699   2.74315682   3.55238806
 6.33504932   0.00000000   3.55238806
 7.91881165  -2.74315682   3.55238806
 9.50257398  -5.48631365   3.55238806
 4.75128699   8.22947047   3.55238806
 6.33504932   5.48631365   3.55238806
 7.91881165   2.74315682   3.55238806
 9.50257398   0.00000000   3.55238806
11.08633632  -2.74315682   3.55238806
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
```

```
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
```

```
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
11.08633632  -0.91438561   1.77619403
12.67009865  -1.82877122   1.77619403
12.67009865  -3.65754243   1.77619403
 7.91881165  11.88701290   1.77619403
 7.91881165  10.05824169   1.77619403
 9.50257398   9.14385608   1.77619403
 9.50257398   7.31508486   1.77619403
11.08633632   6.40069926   1.77619403
11.08633632   4.57192804   1.77619403
12.67009865   3.65754243   1.77619403
12.67009865   1.82877122   1.77619403
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14.25386098  -0.91438561   1.77619403
 1.58376233   0.91438561   5.32858209
 1.58376233  -0.91438561   5.32858209
 3.16752466  -1.82877122   5.32858209
 3.16752466  -3.65754243   5.32858209
 4.75128699  -4.57192804   5.32858209
 4.75128699  -6.40069926   5.32858209
 6.33504932  -7.31508486   5.32858209
 6.33504932  -9.14385608   5.32858209
 7.91881165 -10.05824169   5.32858209
 7.91881165 -11.88701290   5.32858209
 3.16752466   3.65754243   5.32858209
 3.16752466   1.82877122   5.32858209
 4.75128699   0.91438561   5.32858209
 4.75128699  -0.91438561   5.32858209
 6.33504932  -1.82877122   5.32858209
 6.33504932  -3.65754243   5.32858209
 7.91881165  -4.57192804   5.32858209
 7.91881165  -6.40069926   5.32858209
 9.50257398  -7.31508486   5.32858209
 9.50257398  -9.14385608   5.32858209
 4.75128699   6.40069926   5.32858209
 4.75128699   4.57192804   5.32858209
```

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 6.33504932  1.82877122  5.32858209
 7.91881165  0.91438561  5.32858209
 7.91881165 -0.91438561  5.32858209
 9.50257398 -1.82877122  5.32858209
 9.50257398 -3.65754243  5.32858209
11.08633632 -4.57192804  5.32858209
11.08633632 -6.40069926  5.32858209
 6.33504932  9.14385608  5.32858209
 6.33504932  7.31508486  5.32858209
 7.91881165  6.40069926  5.32858209
 7.91881165  4.57192804  5.32858209
 9.50257398  3.65754243  5.32858209
 9.50257398  1.82877122  5.32858209
11.08633632  0.91438561  5.32858209
11.08633632 -0.91438561  5.32858209
12.67009865 -1.82877122  5.32858209
12.67009865 -3.65754243  5.32858209
 7.91881165 11.88701290  5.32858209
 7.91881165 10.05824169  5.32858209
 9.50257398  9.14385608  5.32858209
 9.50257398  7.31508486  5.32858209
11.08633632  6.40069926  5.32858209
11.08633632  4.57192804  5.32858209
12.67009865  3.65754243  5.32858209
12.67009865  1.82877122  5.32858209
14.25386098  0.91438561  5.32858209
14.25386098 -0.91438561  5.32858209
 1.58376233  0.91438561  8.88097015
 1.58376233 -0.91438561  8.88097015
 3.16752466 -1.82877122  8.88097015
 3.16752466 -3.65754243  8.88097015
 4.75128699 -4.57192804  8.88097015
 4.75128699 -6.40069926  8.88097015
 6.33504932 -7.31508486  8.88097015
 6.33504932 -9.14385608  8.88097015
 7.91881165 -10.05824169  8.88097015
 7.91881165 -11.88701290  8.88097015
 3.16752466  3.65754243  8.88097015
 3.16752466  1.82877122  8.88097015
 4.75128699  0.91438561  8.88097015
 4.75128699 -0.91438561  8.88097015
 6.33504932 -1.82877122  8.88097015
 6.33504932 -3.65754243  8.88097015
 7.91881165 -4.57192804  8.88097015
 7.91881165 -6.40069926  8.88097015
 9.50257398 -7.31508486  8.88097015
 9.50257398 -9.14385608  8.88097015
 4.75128699  6.40069926  8.88097015
 4.75128699  4.57192804  8.88097015
 6.33504932  3.65754243  8.88097015
 6.33504932  1.82877122  8.88097015
 7.91881165  0.91438561  8.88097015
 7.91881165 -0.91438561  8.88097015
 9.50257398 -1.82877122  8.88097015
 9.50257398 -3.65754243  8.88097015
11.08633632 -4.57192804  8.88097015
11.08633632 -6.40069926  8.88097015
 6.33504932  9.14385608  8.88097015
 6.33504932  7.31508486  8.88097015
 7.91881165  6.40069926  8.88097015
 7.91881165  4.57192804  8.88097015
```

```
 9.50257398   3.65754243   8.88097015
 9.50257398   1.82877122   8.88097015
11.08633632   0.91438561   8.88097015
11.08633632  -0.91438561   8.88097015
12.67009865  -1.82877122   8.88097015
12.67009865  -3.65754243   8.88097015
 7.91881165  11.88701290   8.88097015
 7.91881165  10.05824169   8.88097015
 9.50257398   9.14385608   8.88097015
 9.50257398   7.31508486   8.88097015
11.08633632   6.40069926   8.88097015
11.08633632   4.57192804   8.88097015
12.67009865   3.65754243   8.88097015
12.67009865   1.82877122   8.88097015
14.25386098   0.91438561   8.88097015
14.25386098  -0.91438561   8.88097015
 1.58376233   0.91438561  12.43335821
 1.58376233  -0.91438561  12.43335821
 3.16752466  -1.82877122  12.43335821
 3.16752466  -3.65754243  12.43335821
 4.75128699  -4.57192804  12.43335821
 4.75128699  -6.40069926  12.43335821
 6.33504932  -7.31508486  12.43335821
 6.33504932  -9.14385608  12.43335821
 7.91881165 -10.05824169  12.43335821
 7.91881165 -11.88701290  12.43335821
 3.16752466   3.65754243  12.43335821
 3.16752466   1.82877122  12.43335821
 4.75128699   0.91438561  12.43335821
 4.75128699  -0.91438561  12.43335821
 6.33504932  -1.82877122  12.43335821
 6.33504932  -3.65754243  12.43335821
 7.91881165  -4.57192804  12.43335821
 7.91881165  -6.40069926  12.43335821
 9.50257398  -7.31508486  12.43335821
 9.50257398  -9.14385608  12.43335821
 4.75128699   6.40069926  12.43335821
 4.75128699   4.57192804  12.43335821
 6.33504932   3.65754243  12.43335821
 6.33504932   1.82877122  12.43335821
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
 9.50257398   1.82877122  12.43335821
11.08633632   0.91438561  12.43335821
11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
12.67009865  -3.65754243  12.43335821
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
```

```
    12.67009865         3.65754243        12.43335821
    12.67009865         1.82877122        12.43335821
    14.25386098         0.91438561        12.43335821
    14.25386098        -0.91438561        12.43335821
     1.58376233         0.91438561        15.98574627
     1.58376233        -0.91438561        15.98574627
     3.16752466        -1.82877122        15.98574627
     3.16752466        -3.65754243        15.98574627
     4.75128699        -4.57192804        15.98574627
     4.75128699        -6.40069926        15.98574627
     6.33504932        -7.31508486        15.98574627
     6.33504932        -9.14385608        15.98574627
     7.91881165       -10.05824169        15.98574627
     7.91881165       -11.88701290        15.98574627
     3.16752466         3.65754243        15.98574627
     3.16752466         1.82877122        15.98574627
     4.75128699         0.91438561        15.98574627
     4.75128699        -0.91438561        15.98574627
     6.33504932        -1.82877122        15.98574627
     6.33504932        -3.65754243        15.98574627
     7.91881165        -4.57192804        15.98574627
     7.91881165        -6.40069926        15.98574627
     9.50257398        -7.31508486        15.98574627
     9.50257398        -9.14385608        15.98574627
     4.75128699         6.40069926        15.98574627
     4.75128699         4.57192804        15.98574627
     6.33504932         3.65754243        15.98574627
     6.33504932         1.82877122        15.98574627
     7.91881165         0.91438561        15.98574627
     7.91881165        -0.91438561        15.98574627
     9.50257398        -1.82877122        15.98574627
     9.50257398        -3.65754243        15.98574627
    11.08633632        -4.57192804        15.98574627
    11.08633632        -6.40069926        15.98574627
     6.33504932         9.14385608        15.98574627
     6.33504932         7.31508486        15.98574627
     7.91881165         6.40069926        15.98574627
     7.91881165         4.57192804        15.98574627
     9.50257398         3.65754243        15.98574627
     9.50257398         1.82877122        15.98574627
    11.08633632         0.91438561        15.98574627
    11.08633632        -0.91438561        15.98574627
    12.67009865        -1.82877122        15.98574627
    12.67009865        -3.65754243        15.98574627
     7.91881165        11.88701290        15.98574627
     7.91881165        10.05824169        15.98574627
     9.50257398         9.14385608        15.98574627
     9.50257398         7.31508486        15.98574627
    11.08633632         6.40069926        15.98574627
    11.08633632         4.57192804        15.98574627
    12.67009865         3.65754243        15.98574627
    12.67009865         1.82877122        15.98574627
    14.25386098         0.91438561        15.98574627
    14.25386098        -0.91438561        15.98574627
  7.91881   0.91439  16.56194
```

Listing 19: Structural input file for configuration: 5x5x5 H B top.

5x5x5_H_B_Zr POSCAR

```
# Zr1 B2
```

```
1.000000
      7.91881165      -13.71578412        0.00000000
      7.91881165       13.71578412        0.00000000
      0.00000000        0.00000000       17.76194030
 Zr   B   H
   125     250     1
Cartesian
      0.00000000        0.00000000        0.00000000
      1.58376233       -2.74315682        0.00000000
      3.16752466       -5.48631365        0.00000000
      4.75128699       -8.22947047        0.00000000
      6.33504932      -10.97262730        0.00000000
      1.58376233        2.74315682        0.00000000
      3.16752466        0.00000000        0.00000000
      4.75128699       -2.74315682        0.00000000
      6.33504932       -5.48631365        0.00000000
      7.91881165       -8.22947047        0.00000000
      3.16752466        5.48631365        0.00000000
      4.75128699        2.74315682        0.00000000
      6.33504932        0.00000000        0.00000000
      7.91881165       -2.74315682        0.00000000
      9.50257398       -5.48631365        0.00000000
      4.75128699        8.22947047        0.00000000
      6.33504932        5.48631365        0.00000000
      7.91881165        2.74315682        0.00000000
      9.50257398        0.00000000        0.00000000
     11.08633632       -2.74315682        0.00000000
      6.33504932       10.97262730        0.00000000
      7.91881165        8.22947047        0.00000000
      9.50257398        5.48631365        0.00000000
     11.08633632        2.74315682        0.00000000
     12.67009865        0.00000000        0.00000000
      0.00000000        0.00000000        3.55238806
      1.58376233       -2.74315682        3.55238806
      3.16752466       -5.48631365        3.55238806
      4.75128699       -8.22947047        3.55238806
      6.33504932      -10.97262730        3.55238806
      1.58376233        2.74315682        3.55238806
      3.16752466        0.00000000        3.55238806
      4.75128699       -2.74315682        3.55238806
      6.33504932       -5.48631365        3.55238806
      7.91881165       -8.22947047        3.55238806
      3.16752466        5.48631365        3.55238806
      4.75128699        2.74315682        3.55238806
      6.33504932        0.00000000        3.55238806
      7.91881165       -2.74315682        3.55238806
      9.50257398       -5.48631365        3.55238806
      4.75128699        8.22947047        3.55238806
      6.33504932        5.48631365        3.55238806
      7.91881165        2.74315682        3.55238806
      9.50257398        0.00000000        3.55238806
     11.08633632       -2.74315682        3.55238806
      6.33504932       10.97262730        3.55238806
      7.91881165        8.22947047        3.55238806
      9.50257398        5.48631365        3.55238806
     11.08633632        2.74315682        3.55238806
     12.67009865        0.00000000        3.55238806
      0.00000000        0.00000000        7.10477612
      1.58376233       -2.74315682        7.10477612
      3.16752466       -5.48631365        7.10477612
      4.75128699       -8.22947047        7.10477612
      6.33504932      -10.97262730        7.10477612
```

```
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
```

```
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
11.08633632  -0.91438561   1.77619403
12.67009865  -1.82877122   1.77619403
12.67009865  -3.65754243   1.77619403
 7.91881165  11.88701290   1.77619403
 7.91881165  10.05824169   1.77619403
 9.50257398   9.14385608   1.77619403
 9.50257398   7.31508486   1.77619403
11.08633632   6.40069926   1.77619403
11.08633632   4.57192804   1.77619403
12.67009865   3.65754243   1.77619403
12.67009865   1.82877122   1.77619403
14.25386098   0.91438561   1.77619403
14.25386098  -0.91438561   1.77619403
 1.58376233   0.91438561   5.32858209
 1.58376233  -0.91438561   5.32858209
 3.16752466  -1.82877122   5.32858209
 3.16752466  -3.65754243   5.32858209
```

```
 4.75128699  -4.57192804  5.32858209
 4.75128699  -6.40069926  5.32858209
 6.33504932  -7.31508486  5.32858209
 6.33504932  -9.14385608  5.32858209
 7.91881165 -10.05824169  5.32858209
 7.91881165 -11.88701290  5.32858209
 3.16752466   3.65754243  5.32858209
 3.16752466   1.82877122  5.32858209
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 4.75128699  -0.91438561  5.32858209
 6.33504932  -1.82877122  5.32858209
 6.33504932  -3.65754243  5.32858209
 7.91881165  -4.57192804  5.32858209
 7.91881165  -6.40069926  5.32858209
 9.50257398  -7.31508486  5.32858209
 9.50257398  -9.14385608  5.32858209
 4.75128699   6.40069926  5.32858209
 4.75128699   4.57192804  5.32858209
 6.33504932   3.65754243  5.32858209
 6.33504932   1.82877122  5.32858209
 7.91881165   0.91438561  5.32858209
 7.91881165  -0.91438561  5.32858209
 9.50257398  -1.82877122  5.32858209
 9.50257398  -3.65754243  5.32858209
11.08633632  -4.57192804  5.32858209
11.08633632  -6.40069926  5.32858209
 6.33504932   9.14385608  5.32858209
 6.33504932   7.31508486  5.32858209
 7.91881165   6.40069926  5.32858209
 7.91881165   4.57192804  5.32858209
 9.50257398   3.65754243  5.32858209
 9.50257398   1.82877122  5.32858209
11.08633632   0.91438561  5.32858209
11.08633632  -0.91438561  5.32858209
12.67009865  -1.82877122  5.32858209
12.67009865  -3.65754243  5.32858209
 7.91881165  11.88701290  5.32858209
 7.91881165  10.05824169  5.32858209
 9.50257398   9.14385608  5.32858209
 9.50257398   7.31508486  5.32858209
11.08633632   6.40069926  5.32858209
11.08633632   4.57192804  5.32858209
12.67009865   3.65754243  5.32858209
12.67009865   1.82877122  5.32858209
14.25386098   0.91438561  5.32858209
14.25386098  -0.91438561  5.32858209
 1.58376233   0.91438561  8.88097015
 1.58376233  -0.91438561  8.88097015
 3.16752466  -1.82877122  8.88097015
 3.16752466  -3.65754243  8.88097015
 4.75128699  -4.57192804  8.88097015
 4.75128699  -6.40069926  8.88097015
 6.33504932  -7.31508486  8.88097015
 6.33504932  -9.14385608  8.88097015
 7.91881165 -10.05824169  8.88097015
 7.91881165 -11.88701290  8.88097015
 3.16752466   3.65754243  8.88097015
 3.16752466   1.82877122  8.88097015
 4.75128699   0.91438561  8.88097015
 4.75128699  -0.91438561  8.88097015
 6.33504932  -1.82877122  8.88097015
 6.33504932  -3.65754243  8.88097015
```

```
 7.91881165       -4.57192804        8.88097015
 7.91881165       -6.40069926        8.88097015
 9.50257398       -7.31508486        8.88097015
 9.50257398       -9.14385608        8.88097015
 4.75128699        6.40069926        8.88097015
 4.75128699        4.57192804        8.88097015
 6.33504932        3.65754243        8.88097015
 6.33504932        1.82877122        8.88097015
 7.91881165        0.91438561        8.88097015
 7.91881165       -0.91438561        8.88097015
 9.50257398       -1.82877122        8.88097015
 9.50257398       -3.65754243        8.88097015
11.08633632       -4.57192804        8.88097015
11.08633632       -6.40069926        8.88097015
 6.33504932        9.14385608        8.88097015
 6.33504932        7.31508486        8.88097015
 7.91881165        6.40069926        8.88097015
 7.91881165        4.57192804        8.88097015
 9.50257398        3.65754243        8.88097015
 9.50257398        1.82877122        8.88097015
11.08633632        0.91438561        8.88097015
11.08633632       -0.91438561        8.88097015
12.67009865       -1.82877122        8.88097015
12.67009865       -3.65754243        8.88097015
 7.91881165       11.88701290        8.88097015
 7.91881165       10.05824169        8.88097015
 9.50257398        9.14385608        8.88097015
 9.50257398        7.31508486        8.88097015
11.08633632        6.40069926        8.88097015
11.08633632        4.57192804        8.88097015
12.67009865        3.65754243        8.88097015
12.67009865        1.82877122        8.88097015
14.25386098        0.91438561        8.88097015
14.25386098       -0.91438561        8.88097015
 1.58376233        0.91438561       12.43335821
 1.58376233       -0.91438561       12.43335821
 3.16752466       -1.82877122       12.43335821
 3.16752466       -3.65754243       12.43335821
 4.75128699       -4.57192804       12.43335821
 4.75128699       -6.40069926       12.43335821
 6.33504932       -7.31508486       12.43335821
 6.33504932       -9.14385608       12.43335821
 7.91881165      -10.05824169       12.43335821
 7.91881165      -11.88701290       12.43335821
 3.16752466        3.65754243       12.43335821
 3.16752466        1.82877122       12.43335821
 4.75128699        0.91438561       12.43335821
 4.75128699       -0.91438561       12.43335821
 6.33504932       -1.82877122       12.43335821
 6.33504932       -3.65754243       12.43335821
 7.91881165       -4.57192804       12.43335821
 7.91881165       -6.40069926       12.43335821
 9.50257398       -7.31508486       12.43335821
 9.50257398       -9.14385608       12.43335821
 4.75128699        6.40069926       12.43335821
 4.75128699        4.57192804       12.43335821
 6.33504932        3.65754243       12.43335821
 6.33504932        1.82877122       12.43335821
 7.91881165        0.91438561       12.43335821
 7.91881165       -0.91438561       12.43335821
 9.50257398       -1.82877122       12.43335821
 9.50257398       -3.65754243       12.43335821
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     11.08633632       -4.57192804       12.43335821
     11.08633632       -6.40069926       12.43335821
      6.33504932        9.14385608       12.43335821
      6.33504932        7.31508486       12.43335821
      7.91881165        6.40069926       12.43335821
      7.91881165        4.57192804       12.43335821
      9.50257398        3.65754243       12.43335821
      9.50257398        1.82877122       12.43335821
     11.08633632        0.91438561       12.43335821
     11.08633632       -0.91438561       12.43335821
     12.67009865       -1.82877122       12.43335821
     12.67009865       -3.65754243       12.43335821
      7.91881165       11.88701290       12.43335821
      7.91881165       10.05824169       12.43335821
      9.50257398        9.14385608       12.43335821
      9.50257398        7.31508486       12.43335821
     11.08633632        6.40069926       12.43335821
     11.08633632        4.57192804       12.43335821
     12.67009865        3.65754243       12.43335821
     12.67009865        1.82877122       12.43335821
     14.25386098        0.91438561       12.43335821
     14.25386098       -0.91438561       12.43335821
      1.58376233        0.91438561       15.98574627
      1.58376233       -0.91438561       15.98574627
      3.16752466       -1.82877122       15.98574627
      3.16752466       -3.65754243       15.98574627
      4.75128699       -4.57192804       15.98574627
      4.75128699       -6.40069926       15.98574627
      6.33504932       -7.31508486       15.98574627
      6.33504932       -9.14385608       15.98574627
      7.91881165      -10.05824169       15.98574627
      7.91881165      -11.88701290       15.98574627
      3.16752466        3.65754243       15.98574627
      3.16752466        1.82877122       15.98574627
      4.75128699        0.91438561       15.98574627
      4.75128699       -0.91438561       15.98574627
      6.33504932       -1.82877122       15.98574627
      6.33504932       -3.65754243       15.98574627
      7.91881165       -4.57192804       15.98574627
      7.91881165       -6.40069926       15.98574627
      9.50257398       -7.31508486       15.98574627
      9.50257398       -9.14385608       15.98574627
      4.75128699        6.40069926       15.98574627
      4.75128699        4.57192804       15.98574627
      6.33504932        3.65754243       15.98574627
      6.33504932        1.82877122       15.98574627
      7.91881165        0.91438561       15.98574627
      7.91881165       -0.91438561       15.98574627
      9.50257398       -1.82877122       15.98574627
      9.50257398       -3.65754243       15.98574627
     11.08633632       -4.57192804       15.98574627
     11.08633632       -6.40069926       15.98574627
      6.33504932        9.14385608       15.98574627
      6.33504932        7.31508486       15.98574627
      7.91881165        6.40069926       15.98574627
      7.91881165        4.57192804       15.98574627
      9.50257398        3.65754243       15.98574627
      9.50257398        1.82877122       15.98574627
     11.08633632        0.91438561       15.98574627
     11.08633632       -0.91438561       15.98574627
     12.67009865       -1.82877122       15.98574627
     12.67009865       -3.65754243       15.98574627
```

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      7.91881165       11.88701290       15.98574627
      7.91881165       10.05824169       15.98574627
      9.50257398        9.14385608       15.98574627
      9.50257398        7.31508486       15.98574627
     11.08633632        6.40069926       15.98574627
     11.08633632        4.57192804       15.98574627
     12.67009865        3.65754243       15.98574627
     12.67009865        1.82877122       15.98574627
     14.25386098        0.91438561       15.98574627
     14.25386098       -0.91438561       15.98574627
   7.91881   1.8439  16.8194
```

Listing 20: Structural input file for configuration: 5x5x5 H B Zr.

5x5x5_H_triangle POSCAR

```
# Zr1 B2
1.000000
      7.91881165      -13.71578412        0.00000000
      7.91881165       13.71578412        0.00000000
      0.00000000        0.00000000       17.76194030
 Zr  B  H
   125     250     1
Cartesian
      0.00000000        0.00000000        0.00000000
      1.58376233       -2.74315682        0.00000000
      3.16752466       -5.48631365        0.00000000
      4.75128699       -8.22947047        0.00000000
      6.33504932      -10.97262730        0.00000000
      1.58376233        2.74315682        0.00000000
      3.16752466        0.00000000        0.00000000
      4.75128699       -2.74315682        0.00000000
      6.33504932       -5.48631365        0.00000000
      7.91881165       -8.22947047        0.00000000
      3.16752466        5.48631365        0.00000000
      4.75128699        2.74315682        0.00000000
      6.33504932        0.00000000        0.00000000
      7.91881165       -2.74315682        0.00000000
      9.50257398       -5.48631365        0.00000000
      4.75128699        8.22947047        0.00000000
      6.33504932        5.48631365        0.00000000
      7.91881165        2.74315682        0.00000000
      9.50257398        0.00000000        0.00000000
     11.08633632       -2.74315682        0.00000000
      6.33504932       10.97262730        0.00000000
      7.91881165        8.22947047        0.00000000
      9.50257398        5.48631365        0.00000000
     11.08633632        2.74315682        0.00000000
     12.67009865        0.00000000        0.00000000
      0.00000000        0.00000000        3.55238806
      1.58376233       -2.74315682        3.55238806
      3.16752466       -5.48631365        3.55238806
      4.75128699       -8.22947047        3.55238806
      6.33504932      -10.97262730        3.55238806
      1.58376233        2.74315682        3.55238806
      3.16752466        0.00000000        3.55238806
      4.75128699       -2.74315682        3.55238806
      6.33504932       -5.48631365        3.55238806
      7.91881165       -8.22947047        3.55238806
      3.16752466        5.48631365        3.55238806
      4.75128699        2.74315682        3.55238806
```

```
 6.33504932   0.00000000   3.55238806
 7.91881165  -2.74315682   3.55238806
 9.50257398  -5.48631365   3.55238806
 4.75128699   8.22947047   3.55238806
 6.33504932   5.48631365   3.55238806
 7.91881165   2.74315682   3.55238806
 9.50257398   0.00000000   3.55238806
11.08633632  -2.74315682   3.55238806
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
```

```
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
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 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
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 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
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 12.67009865  -3.65754243   1.77619403
  7.91881165  11.88701290   1.77619403
  7.91881165  10.05824169   1.77619403
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  9.50257398   7.31508486   1.77619403
 11.08633632   6.40069926   1.77619403
 11.08633632   4.57192804   1.77619403
 12.67009865   3.65754243   1.77619403
 12.67009865   1.82877122   1.77619403
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 14.25386098  -0.91438561   1.77619403
  1.58376233   0.91438561   5.32858209
  1.58376233  -0.91438561   5.32858209
  3.16752466  -1.82877122   5.32858209
  3.16752466  -3.65754243   5.32858209
  4.75128699  -4.57192804   5.32858209
  4.75128699  -6.40069926   5.32858209
  6.33504932  -7.31508486   5.32858209
  6.33504932  -9.14385608   5.32858209
  7.91881165 -10.05824169   5.32858209
  7.91881165 -11.88701290   5.32858209
  3.16752466   3.65754243   5.32858209
  3.16752466   1.82877122   5.32858209
  4.75128699   0.91438561   5.32858209
  4.75128699  -0.91438561   5.32858209
  6.33504932  -1.82877122   5.32858209
  6.33504932  -3.65754243   5.32858209
  7.91881165  -4.57192804   5.32858209
  7.91881165  -6.40069926   5.32858209
  9.50257398  -7.31508486   5.32858209
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  4.75128699   4.57192804   5.32858209
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  6.33504932   1.82877122   5.32858209
  7.91881165   0.91438561   5.32858209
  7.91881165  -0.91438561   5.32858209
  9.50257398  -1.82877122   5.32858209
  9.50257398  -3.65754243   5.32858209
 11.08633632  -4.57192804   5.32858209
 11.08633632  -6.40069926   5.32858209
  6.33504932   9.14385608   5.32858209
  6.33504932   7.31508486   5.32858209
  7.91881165   6.40069926   5.32858209
  7.91881165   4.57192804   5.32858209
  9.50257398   3.65754243   5.32858209
  9.50257398   1.82877122   5.32858209
 11.08633632   0.91438561   5.32858209
 11.08633632  -0.91438561   5.32858209
 12.67009865  -1.82877122   5.32858209
 12.67009865  -3.65754243   5.32858209
  7.91881165  11.88701290   5.32858209
  7.91881165  10.05824169   5.32858209
  9.50257398   9.14385608   5.32858209
  9.50257398   7.31508486   5.32858209
 11.08633632   6.40069926   5.32858209
 11.08633632   4.57192804   5.32858209
 12.67009865   3.65754243   5.32858209
 12.67009865   1.82877122   5.32858209
```

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14.25386098  -0.91438561   5.32858209
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 1.58376233  -0.91438561   8.88097015
 3.16752466  -1.82877122   8.88097015
 3.16752466  -3.65754243   8.88097015
 4.75128699  -4.57192804   8.88097015
 4.75128699  -6.40069926   8.88097015
 6.33504932  -7.31508486   8.88097015
 6.33504932  -9.14385608   8.88097015
 7.91881165 -10.05824169   8.88097015
 7.91881165 -11.88701290   8.88097015
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 4.75128699  -0.91438561   8.88097015
 6.33504932  -1.82877122   8.88097015
 6.33504932  -3.65754243   8.88097015
 7.91881165  -4.57192804   8.88097015
 7.91881165  -6.40069926   8.88097015
 9.50257398  -7.31508486   8.88097015
 9.50257398  -9.14385608   8.88097015
 4.75128699   6.40069926   8.88097015
 4.75128699   4.57192804   8.88097015
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 7.91881165  -0.91438561   8.88097015
 9.50257398  -1.82877122   8.88097015
 9.50257398  -3.65754243   8.88097015
11.08633632  -4.57192804   8.88097015
11.08633632  -6.40069926   8.88097015
 6.33504932   9.14385608   8.88097015
 6.33504932   7.31508486   8.88097015
 7.91881165   6.40069926   8.88097015
 7.91881165   4.57192804   8.88097015
 9.50257398   3.65754243   8.88097015
 9.50257398   1.82877122   8.88097015
11.08633632   0.91438561   8.88097015
11.08633632  -0.91438561   8.88097015
12.67009865  -1.82877122   8.88097015
12.67009865  -3.65754243   8.88097015
 7.91881165  11.88701290   8.88097015
 7.91881165  10.05824169   8.88097015
 9.50257398   9.14385608   8.88097015
 9.50257398   7.31508486   8.88097015
11.08633632   6.40069926   8.88097015
11.08633632   4.57192804   8.88097015
12.67009865   3.65754243   8.88097015
12.67009865   1.82877122   8.88097015
14.25386098   0.91438561   8.88097015
14.25386098  -0.91438561   8.88097015
 1.58376233   0.91438561  12.43335821
 1.58376233  -0.91438561  12.43335821
 3.16752466  -1.82877122  12.43335821
 3.16752466  -3.65754243  12.43335821
 4.75128699  -4.57192804  12.43335821
 4.75128699  -6.40069926  12.43335821
 6.33504932  -7.31508486  12.43335821
 6.33504932  -9.14385608  12.43335821
 7.91881165 -10.05824169  12.43335821
 7.91881165 -11.88701290  12.43335821
```

```
 3.16752466  3.65754243  12.43335821
 3.16752466  1.82877122  12.43335821
 4.75128699  0.91438561  12.43335821
 4.75128699 -0.91438561  12.43335821
 6.33504932 -1.82877122  12.43335821
 6.33504932 -3.65754243  12.43335821
 7.91881165 -4.57192804  12.43335821
 7.91881165 -6.40069926  12.43335821
 9.50257398 -7.31508486  12.43335821
 9.50257398 -9.14385608  12.43335821
 4.75128699  6.40069926  12.43335821
 4.75128699  4.57192804  12.43335821
 6.33504932  3.65754243  12.43335821
 6.33504932  1.82877122  12.43335821
 7.91881165  0.91438561  12.43335821
 7.91881165 -0.91438561  12.43335821
 9.50257398 -1.82877122  12.43335821
 9.50257398 -3.65754243  12.43335821
11.08633632 -4.57192804  12.43335821
11.08633632 -6.40069926  12.43335821
 6.33504932  9.14385608  12.43335821
 6.33504932  7.31508486  12.43335821
 7.91881165  6.40069926  12.43335821
 7.91881165  4.57192804  12.43335821
 9.50257398  3.65754243  12.43335821
 9.50257398  1.82877122  12.43335821
11.08633632  0.91438561  12.43335821
11.08633632 -0.91438561  12.43335821
12.67009865 -1.82877122  12.43335821
12.67009865 -3.65754243  12.43335821
 7.91881165 11.88701290  12.43335821
 7.91881165 10.05824169  12.43335821
 9.50257398  9.14385608  12.43335821
 9.50257398  7.31508486  12.43335821
11.08633632  6.40069926  12.43335821
11.08633632  4.57192804  12.43335821
12.67009865  3.65754243  12.43335821
12.67009865  1.82877122  12.43335821
14.25386098  0.91438561  12.43335821
14.25386098 -0.91438561  12.43335821
 1.58376233  0.91438561  15.98574627
 1.58376233 -0.91438561  15.98574627
 3.16752466 -1.82877122  15.98574627
 3.16752466 -3.65754243  15.98574627
 4.75128699 -4.57192804  15.98574627
 4.75128699 -6.40069926  15.98574627
 6.33504932 -7.31508486  15.98574627
 6.33504932 -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466  3.65754243  15.98574627
 3.16752466  1.82877122  15.98574627
 4.75128699  0.91438561  15.98574627
 4.75128699 -0.91438561  15.98574627
 6.33504932 -1.82877122  15.98574627
 6.33504932 -3.65754243  15.98574627
 7.91881165 -4.57192804  15.98574627
 7.91881165 -6.40069926  15.98574627
 9.50257398 -7.31508486  15.98574627
 9.50257398 -9.14385608  15.98574627
 4.75128699  6.40069926  15.98574627
 4.75128699  4.57192804  15.98574627
```

```
      6.33504932         3.65754243        15.98574627
      6.33504932         1.82877122        15.98574627
      7.91881165         0.91438561        15.98574627
      7.91881165        -0.91438561        15.98574627
      9.50257398        -1.82877122        15.98574627
      9.50257398        -3.65754243        15.98574627
     11.08633632        -4.57192804        15.98574627
     11.08633632        -6.40069926        15.98574627
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   8.6   1.7  15.98575
```

Listing 21: Structural input file for configuration: 5x5x5 H triangle.

5x5x5_H_Zr_ring POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr   B   H
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
      4.75128699         8.22947047         0.00000000
      6.33504932         5.48631365         0.00000000
      7.91881165         2.74315682         0.00000000
      9.50257398         0.00000000         0.00000000
```

```
11.08633632  -2.74315682   0.00000000
 6.33504932  10.97262730   0.00000000
 7.91881165   8.22947047   0.00000000
 9.50257398   5.48631365   0.00000000
11.08633632   2.74315682   0.00000000
12.67009865   0.00000000   0.00000000
 0.00000000   0.00000000   3.55238806
 1.58376233  -2.74315682   3.55238806
 3.16752466  -5.48631365   3.55238806
 4.75128699  -8.22947047   3.55238806
 6.33504932 -10.97262730   3.55238806
 1.58376233   2.74315682   3.55238806
 3.16752466   0.00000000   3.55238806
 4.75128699  -2.74315682   3.55238806
 6.33504932  -5.48631365   3.55238806
 7.91881165  -8.22947047   3.55238806
 3.16752466   5.48631365   3.55238806
 4.75128699   2.74315682   3.55238806
 6.33504932   0.00000000   3.55238806
 7.91881165  -2.74315682   3.55238806
 9.50257398  -5.48631365   3.55238806
 4.75128699   8.22947047   3.55238806
 6.33504932   5.48631365   3.55238806
 7.91881165   2.74315682   3.55238806
 9.50257398   0.00000000   3.55238806
11.08633632  -2.74315682   3.55238806
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
```

```
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
```

```
 9.50257398  -7.31508486  1.77619403
 9.50257398  -9.14385608  1.77619403
 4.75128699   6.40069926  1.77619403
 4.75128699   4.57192804  1.77619403
 6.33504932   3.65754243  1.77619403
 6.33504932   1.82877122  1.77619403
 7.91881165   0.91438561  1.77619403
 7.91881165  -0.91438561  1.77619403
 9.50257398  -1.82877122  1.77619403
 9.50257398  -3.65754243  1.77619403
11.08633632  -4.57192804  1.77619403
11.08633632  -6.40069926  1.77619403
 6.33504932   9.14385608  1.77619403
 6.33504932   7.31508486  1.77619403
 7.91881165   6.40069926  1.77619403
 7.91881165   4.57192804  1.77619403
 9.50257398   3.65754243  1.77619403
 9.50257398   1.82877122  1.77619403
11.08633632   0.91438561  1.77619403
11.08633632  -0.91438561  1.77619403
12.67009865  -1.82877122  1.77619403
12.67009865  -3.65754243  1.77619403
 7.91881165  11.88701290  1.77619403
 7.91881165  10.05824169  1.77619403
 9.50257398   9.14385608  1.77619403
 9.50257398   7.31508486  1.77619403
11.08633632   6.40069926  1.77619403
11.08633632   4.57192804  1.77619403
12.67009865   3.65754243  1.77619403
12.67009865   1.82877122  1.77619403
14.25386098   0.91438561  1.77619403
14.25386098  -0.91438561  1.77619403
 1.58376233   0.91438561  5.32858209
 1.58376233  -0.91438561  5.32858209
 3.16752466  -1.82877122  5.32858209
 3.16752466  -3.65754243  5.32858209
 4.75128699  -4.57192804  5.32858209
 4.75128699  -6.40069926  5.32858209
 6.33504932  -7.31508486  5.32858209
 6.33504932  -9.14385608  5.32858209
 7.91881165 -10.05824169  5.32858209
 7.91881165 -11.88701290  5.32858209
 3.16752466   3.65754243  5.32858209
 3.16752466   1.82877122  5.32858209
 4.75128699   0.91438561  5.32858209
 4.75128699  -0.91438561  5.32858209
 6.33504932  -1.82877122  5.32858209
 6.33504932  -3.65754243  5.32858209
 7.91881165  -4.57192804  5.32858209
 7.91881165  -6.40069926  5.32858209
 9.50257398  -7.31508486  5.32858209
 9.50257398  -9.14385608  5.32858209
 4.75128699   6.40069926  5.32858209
 4.75128699   4.57192804  5.32858209
 6.33504932   3.65754243  5.32858209
 6.33504932   1.82877122  5.32858209
 7.91881165   0.91438561  5.32858209
 7.91881165  -0.91438561  5.32858209
 9.50257398  -1.82877122  5.32858209
 9.50257398  -3.65754243  5.32858209
11.08633632  -4.57192804  5.32858209
11.08633632  -6.40069926  5.32858209
```

```
 6.33504932   9.14385608   5.32858209
 6.33504932   7.31508486   5.32858209
 7.91881165   6.40069926   5.32858209
 7.91881165   4.57192804   5.32858209
 9.50257398   3.65754243   5.32858209
 9.50257398   1.82877122   5.32858209
11.08633632   0.91438561   5.32858209
11.08633632  -0.91438561   5.32858209
12.67009865  -1.82877122   5.32858209
12.67009865  -3.65754243   5.32858209
 7.91881165  11.88701290   5.32858209
 7.91881165  10.05824169   5.32858209
 9.50257398   9.14385608   5.32858209
 9.50257398   7.31508486   5.32858209
11.08633632   6.40069926   5.32858209
11.08633632   4.57192804   5.32858209
12.67009865   3.65754243   5.32858209
12.67009865   1.82877122   5.32858209
14.25386098   0.91438561   5.32858209
14.25386098  -0.91438561   5.32858209
 1.58376233   0.91438561   8.88097015
 1.58376233  -0.91438561   8.88097015
 3.16752466  -1.82877122   8.88097015
 3.16752466  -3.65754243   8.88097015
 4.75128699  -4.57192804   8.88097015
 4.75128699  -6.40069926   8.88097015
 6.33504932  -7.31508486   8.88097015
 6.33504932  -9.14385608   8.88097015
 7.91881165 -10.05824169   8.88097015
 7.91881165 -11.88701290   8.88097015
 3.16752466   3.65754243   8.88097015
 3.16752466   1.82877122   8.88097015
 4.75128699   0.91438561   8.88097015
 4.75128699  -0.91438561   8.88097015
 6.33504932  -1.82877122   8.88097015
 6.33504932  -3.65754243   8.88097015
 7.91881165  -4.57192804   8.88097015
 7.91881165  -6.40069926   8.88097015
 9.50257398  -7.31508486   8.88097015
 9.50257398  -9.14385608   8.88097015
 4.75128699   6.40069926   8.88097015
 4.75128699   4.57192804   8.88097015
 6.33504932   3.65754243   8.88097015
 6.33504932   1.82877122   8.88097015
 7.91881165   0.91438561   8.88097015
 7.91881165  -0.91438561   8.88097015
 9.50257398  -1.82877122   8.88097015
 9.50257398  -3.65754243   8.88097015
11.08633632  -4.57192804   8.88097015
11.08633632  -6.40069926   8.88097015
 6.33504932   9.14385608   8.88097015
 6.33504932   7.31508486   8.88097015
 7.91881165   6.40069926   8.88097015
 7.91881165   4.57192804   8.88097015
 9.50257398   3.65754243   8.88097015
 9.50257398   1.82877122   8.88097015
11.08633632   0.91438561   8.88097015
11.08633632  -0.91438561   8.88097015
12.67009865  -1.82877122   8.88097015
12.67009865  -3.65754243   8.88097015
 7.91881165  11.88701290   8.88097015
 7.91881165  10.05824169   8.88097015
```

```
 9.50257398   9.14385608   8.88097015
 9.50257398   7.31508486   8.88097015
11.08633632   6.40069926   8.88097015
11.08633632   4.57192804   8.88097015
12.67009865   3.65754243   8.88097015
12.67009865   1.82877122   8.88097015
14.25386098   0.91438561   8.88097015
14.25386098  -0.91438561   8.88097015
 1.58376233   0.91438561  12.43335821
 1.58376233  -0.91438561  12.43335821
 3.16752466  -1.82877122  12.43335821
 3.16752466  -3.65754243  12.43335821
 4.75128699  -4.57192804  12.43335821
 4.75128699  -6.40069926  12.43335821
 6.33504932  -7.31508486  12.43335821
 6.33504932  -9.14385608  12.43335821
 7.91881165 -10.05824169  12.43335821
 7.91881165 -11.88701290  12.43335821
 3.16752466   3.65754243  12.43335821
 3.16752466   1.82877122  12.43335821
 4.75128699   0.91438561  12.43335821
 4.75128699  -0.91438561  12.43335821
 6.33504932  -1.82877122  12.43335821
 6.33504932  -3.65754243  12.43335821
 7.91881165  -4.57192804  12.43335821
 7.91881165  -6.40069926  12.43335821
 9.50257398  -7.31508486  12.43335821
 9.50257398  -9.14385608  12.43335821
 4.75128699   6.40069926  12.43335821
 4.75128699   4.57192804  12.43335821
 6.33504932   3.65754243  12.43335821
 6.33504932   1.82877122  12.43335821
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
 9.50257398   1.82877122  12.43335821
11.08633632   0.91438561  12.43335821
11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
12.67009865  -3.65754243  12.43335821
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
```

```
      4.75128699        -4.57192804        15.98574627
      4.75128699        -6.40069926        15.98574627
      6.33504932        -7.31508486        15.98574627
      6.33504932        -9.14385608        15.98574627
      7.91881165       -10.05824169        15.98574627
      7.91881165       -11.88701290        15.98574627
      3.16752466         3.65754243        15.98574627
      3.16752466         1.82877122        15.98574627
      4.75128699         0.91438561        15.98574627
      4.75128699        -0.91438561        15.98574627
      6.33504932        -1.82877122        15.98574627
      6.33504932        -3.65754243        15.98574627
      7.91881165        -4.57192804        15.98574627
      7.91881165        -6.40069926        15.98574627
      9.50257398        -7.31508486        15.98574627
      9.50257398        -9.14385608        15.98574627
      4.75128699         6.40069926        15.98574627
      4.75128699         4.57192804        15.98574627
      6.33504932         3.65754243        15.98574627
      6.33504932         1.82877122        15.98574627
      7.91881165         0.91438561        15.98574627
      7.91881165        -0.91438561        15.98574627
      9.50257398        -1.82877122        15.98574627
      9.50257398        -3.65754243        15.98574627
     11.08633632        -4.57192804        15.98574627
     11.08633632        -6.40069926        15.98574627
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   7.91881    0.91439   17.76194
```

Listing 22: Structural input file for configuration: 5x5x5 H Zr ring.

5x5x5_H_Zr_top POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr  B  H
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
```

```
 1.58376233  -2.74315682  0.00000000
 3.16752466  -5.48631365  0.00000000
 4.75128699  -8.22947047  0.00000000
 6.33504932 -10.97262730  0.00000000
 1.58376233   2.74315682  0.00000000
 3.16752466   0.00000000  0.00000000
 4.75128699  -2.74315682  0.00000000
 6.33504932  -5.48631365  0.00000000
 7.91881165  -8.22947047  0.00000000
 3.16752466   5.48631365  0.00000000
 4.75128699   2.74315682  0.00000000
 6.33504932   0.00000000  0.00000000
 7.91881165  -2.74315682  0.00000000
 9.50257398  -5.48631365  0.00000000
 4.75128699   8.22947047  0.00000000
 6.33504932   5.48631365  0.00000000
 7.91881165   2.74315682  0.00000000
 9.50257398   0.00000000  0.00000000
11.08633632  -2.74315682  0.00000000
 6.33504932  10.97262730  0.00000000
 7.91881165   8.22947047  0.00000000
 9.50257398   5.48631365  0.00000000
11.08633632   2.74315682  0.00000000
12.67009865   0.00000000  0.00000000
 0.00000000   0.00000000  3.55238806
 1.58376233  -2.74315682  3.55238806
 3.16752466  -5.48631365  3.55238806
 4.75128699  -8.22947047  3.55238806
 6.33504932 -10.97262730  3.55238806
 1.58376233   2.74315682  3.55238806
 3.16752466   0.00000000  3.55238806
 4.75128699  -2.74315682  3.55238806
 6.33504932  -5.48631365  3.55238806
 7.91881165  -8.22947047  3.55238806
 3.16752466   5.48631365  3.55238806
 4.75128699   2.74315682  3.55238806
 6.33504932   0.00000000  3.55238806
 7.91881165  -2.74315682  3.55238806
 9.50257398  -5.48631365  3.55238806
 4.75128699   8.22947047  3.55238806
 6.33504932   5.48631365  3.55238806
 7.91881165   2.74315682  3.55238806
 9.50257398   0.00000000  3.55238806
11.08633632  -2.74315682  3.55238806
 6.33504932  10.97262730  3.55238806
 7.91881165   8.22947047  3.55238806
 9.50257398   5.48631365  3.55238806
11.08633632   2.74315682  3.55238806
12.67009865   0.00000000  3.55238806
 0.00000000   0.00000000  7.10477612
 1.58376233  -2.74315682  7.10477612
 3.16752466  -5.48631365  7.10477612
 4.75128699  -8.22947047  7.10477612
 6.33504932 -10.97262730  7.10477612
 1.58376233   2.74315682  7.10477612
 3.16752466   0.00000000  7.10477612
 4.75128699  -2.74315682  7.10477612
 6.33504932  -5.48631365  7.10477612
 7.91881165  -8.22947047  7.10477612
 3.16752466   5.48631365  7.10477612
 4.75128699   2.74315682  7.10477612
 6.33504932   0.00000000  7.10477612
```

```
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
```

```
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
11.08633632  -0.91438561   1.77619403
12.67009865  -1.82877122   1.77619403
12.67009865  -3.65754243   1.77619403
 7.91881165  11.88701290   1.77619403
 7.91881165  10.05824169   1.77619403
 9.50257398   9.14385608   1.77619403
 9.50257398   7.31508486   1.77619403
11.08633632   6.40069926   1.77619403
11.08633632   4.57192804   1.77619403
12.67009865   3.65754243   1.77619403
12.67009865   1.82877122   1.77619403
14.25386098   0.91438561   1.77619403
14.25386098  -0.91438561   1.77619403
 1.58376233   0.91438561   5.32858209
 1.58376233  -0.91438561   5.32858209
 3.16752466  -1.82877122   5.32858209
 3.16752466  -3.65754243   5.32858209
 4.75128699  -4.57192804   5.32858209
 4.75128699  -6.40069926   5.32858209
 6.33504932  -7.31508486   5.32858209
 6.33504932  -9.14385608   5.32858209
 7.91881165 -10.05824169   5.32858209
 7.91881165 -11.88701290   5.32858209
 3.16752466   3.65754243   5.32858209
 3.16752466   1.82877122   5.32858209
```

```
 4.75128699  0.91438561  5.32858209
 4.75128699 -0.91438561  5.32858209
 6.33504932 -1.82877122  5.32858209
 6.33504932 -3.65754243  5.32858209
 7.91881165 -4.57192804  5.32858209
 7.91881165 -6.40069926  5.32858209
 9.50257398 -7.31508486  5.32858209
 9.50257398 -9.14385608  5.32858209
 4.75128699  6.40069926  5.32858209
 4.75128699  4.57192804  5.32858209
 6.33504932  3.65754243  5.32858209
 6.33504932  1.82877122  5.32858209
 7.91881165  0.91438561  5.32858209
 7.91881165 -0.91438561  5.32858209
 9.50257398 -1.82877122  5.32858209
 9.50257398 -3.65754243  5.32858209
11.08633632 -4.57192804  5.32858209
11.08633632 -6.40069926  5.32858209
 6.33504932  9.14385608  5.32858209
 6.33504932  7.31508486  5.32858209
 7.91881165  6.40069926  5.32858209
 7.91881165  4.57192804  5.32858209
 9.50257398  3.65754243  5.32858209
 9.50257398  1.82877122  5.32858209
11.08633632  0.91438561  5.32858209
11.08633632 -0.91438561  5.32858209
12.67009865 -1.82877122  5.32858209
12.67009865 -3.65754243  5.32858209
 7.91881165 11.88701290  5.32858209
 7.91881165 10.05824169  5.32858209
 9.50257398  9.14385608  5.32858209
 9.50257398  7.31508486  5.32858209
11.08633632  6.40069926  5.32858209
11.08633632  4.57192804  5.32858209
12.67009865  3.65754243  5.32858209
12.67009865  1.82877122  5.32858209
14.25386098  0.91438561  5.32858209
14.25386098 -0.91438561  5.32858209
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 1.58376233 -0.91438561  8.88097015
 3.16752466 -1.82877122  8.88097015
 3.16752466 -3.65754243  8.88097015
 4.75128699 -4.57192804  8.88097015
 4.75128699 -6.40069926  8.88097015
 6.33504932 -7.31508486  8.88097015
 6.33504932 -9.14385608  8.88097015
 7.91881165 -10.05824169  8.88097015
 7.91881165 -11.88701290  8.88097015
 3.16752466  3.65754243  8.88097015
 3.16752466  1.82877122  8.88097015
 4.75128699  0.91438561  8.88097015
 4.75128699 -0.91438561  8.88097015
 6.33504932 -1.82877122  8.88097015
 6.33504932 -3.65754243  8.88097015
 7.91881165 -4.57192804  8.88097015
 7.91881165 -6.40069926  8.88097015
 9.50257398 -7.31508486  8.88097015
 9.50257398 -9.14385608  8.88097015
 4.75128699  6.40069926  8.88097015
 4.75128699  4.57192804  8.88097015
 6.33504932  3.65754243  8.88097015
 6.33504932  1.82877122  8.88097015
```

```
 7.91881165  0.91438561  8.88097015
 7.91881165 -0.91438561  8.88097015
 9.50257398 -1.82877122  8.88097015
 9.50257398 -3.65754243  8.88097015
11.08633632 -4.57192804  8.88097015
11.08633632 -6.40069926  8.88097015
 6.33504932  9.14385608  8.88097015
 6.33504932  7.31508486  8.88097015
 7.91881165  6.40069926  8.88097015
 7.91881165  4.57192804  8.88097015
 9.50257398  3.65754243  8.88097015
 9.50257398  1.82877122  8.88097015
11.08633632  0.91438561  8.88097015
11.08633632 -0.91438561  8.88097015
12.67009865 -1.82877122  8.88097015
12.67009865 -3.65754243  8.88097015
 7.91881165 11.88701290  8.88097015
 7.91881165 10.05824169  8.88097015
 9.50257398  9.14385608  8.88097015
 9.50257398  7.31508486  8.88097015
11.08633632  6.40069926  8.88097015
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12.67009865  3.65754243  8.88097015
12.67009865  1.82877122  8.88097015
14.25386098  0.91438561  8.88097015
14.25386098 -0.91438561  8.88097015
 1.58376233  0.91438561 12.43335821
 1.58376233 -0.91438561 12.43335821
 3.16752466 -1.82877122 12.43335821
 3.16752466 -3.65754243 12.43335821
 4.75128699 -4.57192804 12.43335821
 4.75128699 -6.40069926 12.43335821
 6.33504932 -7.31508486 12.43335821
 6.33504932 -9.14385608 12.43335821
 7.91881165 -10.05824169 12.43335821
 7.91881165 -11.88701290 12.43335821
 3.16752466  3.65754243 12.43335821
 3.16752466  1.82877122 12.43335821
 4.75128699  0.91438561 12.43335821
 4.75128699 -0.91438561 12.43335821
 6.33504932 -1.82877122 12.43335821
 6.33504932 -3.65754243 12.43335821
 7.91881165 -4.57192804 12.43335821
 7.91881165 -6.40069926 12.43335821
 9.50257398 -7.31508486 12.43335821
 9.50257398 -9.14385608 12.43335821
 4.75128699  6.40069926 12.43335821
 4.75128699  4.57192804 12.43335821
 6.33504932  3.65754243 12.43335821
 6.33504932  1.82877122 12.43335821
 7.91881165  0.91438561 12.43335821
 7.91881165 -0.91438561 12.43335821
 9.50257398 -1.82877122 12.43335821
 9.50257398 -3.65754243 12.43335821
11.08633632 -4.57192804 12.43335821
11.08633632 -6.40069926 12.43335821
 6.33504932  9.14385608 12.43335821
 6.33504932  7.31508486 12.43335821
 7.91881165  6.40069926 12.43335821
 7.91881165  4.57192804 12.43335821
 9.50257398  3.65754243 12.43335821
 9.50257398  1.82877122 12.43335821
```

```
 11.08633632   0.91438561  12.43335821
 11.08633632  -0.91438561  12.43335821
 12.67009865  -1.82877122  12.43335821
 12.67009865  -3.65754243  12.43335821
  7.91881165  11.88701290  12.43335821
  7.91881165  10.05824169  12.43335821
  9.50257398   9.14385608  12.43335821
  9.50257398   7.31508486  12.43335821
 11.08633632   6.40069926  12.43335821
 11.08633632   4.57192804  12.43335821
 12.67009865   3.65754243  12.43335821
 12.67009865   1.82877122  12.43335821
 14.25386098   0.91438561  12.43335821
 14.25386098  -0.91438561  12.43335821
  1.58376233   0.91438561  15.98574627
  1.58376233  -0.91438561  15.98574627
  3.16752466  -1.82877122  15.98574627
  3.16752466  -3.65754243  15.98574627
  4.75128699  -4.57192804  15.98574627
  4.75128699  -6.40069926  15.98574627
  6.33504932  -7.31508486  15.98574627
  6.33504932  -9.14385608  15.98574627
  7.91881165 -10.05824169  15.98574627
  7.91881165 -11.88701290  15.98574627
  3.16752466   3.65754243  15.98574627
  3.16752466   1.82877122  15.98574627
  4.75128699   0.91438561  15.98574627
  4.75128699  -0.91438561  15.98574627
  6.33504932  -1.82877122  15.98574627
  6.33504932  -3.65754243  15.98574627
  7.91881165  -4.57192804  15.98574627
  7.91881165  -6.40069926  15.98574627
  9.50257398  -7.31508486  15.98574627
  9.50257398  -9.14385608  15.98574627
  4.75128699   6.40069926  15.98574627
  4.75128699   4.57192804  15.98574627
  6.33504932   3.65754243  15.98574627
  6.33504932   1.82877122  15.98574627
  7.91881165   0.91438561  15.98574627
  7.91881165  -0.91438561  15.98574627
  9.50257398  -1.82877122  15.98574627
  9.50257398  -3.65754243  15.98574627
 11.08633632  -4.57192804  15.98574627
 11.08633632  -6.40069926  15.98574627
  6.33504932   9.14385608  15.98574627
  6.33504932   7.31508486  15.98574627
  7.91881165   6.40069926  15.98574627
  7.91881165   4.57192804  15.98574627
  9.50257398   3.65754243  15.98574627
  9.50257398   1.82877122  15.98574627
 11.08633632   0.91438561  15.98574627
 11.08633632  -0.91438561  15.98574627
 12.67009865  -1.82877122  15.98574627
 12.67009865  -3.65754243  15.98574627
  7.91881165  11.88701290  15.98574627
  7.91881165  10.05824169  15.98574627
  9.50257398   9.14385608  15.98574627
  9.50257398   7.31508486  15.98574627
 11.08633632   6.40069926  15.98574627
 11.08633632   4.57192804  15.98574627
 12.67009865   3.65754243  15.98574627
 12.67009865   1.82877122  15.98574627
```

```
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   6.33505   0   16.98575
```

Listing 23: Structural input file for configuration: 5x5x5 H Zr top.

5x5x5_N_B_top POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr   B   N
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
      4.75128699         8.22947047         0.00000000
      6.33504932         5.48631365         0.00000000
      7.91881165         2.74315682         0.00000000
      9.50257398         0.00000000         0.00000000
     11.08633632        -2.74315682         0.00000000
      6.33504932        10.97262730         0.00000000
      7.91881165         8.22947047         0.00000000
      9.50257398         5.48631365         0.00000000
     11.08633632         2.74315682         0.00000000
     12.67009865         0.00000000         0.00000000
      0.00000000         0.00000000         3.55238806
      1.58376233        -2.74315682         3.55238806
      3.16752466        -5.48631365         3.55238806
      4.75128699        -8.22947047         3.55238806
      6.33504932       -10.97262730         3.55238806
      1.58376233         2.74315682         3.55238806
      3.16752466         0.00000000         3.55238806
      4.75128699        -2.74315682         3.55238806
      6.33504932        -5.48631365         3.55238806
      7.91881165        -8.22947047         3.55238806
      3.16752466         5.48631365         3.55238806
      4.75128699         2.74315682         3.55238806
      6.33504932         0.00000000         3.55238806
      7.91881165        -2.74315682         3.55238806
      9.50257398        -5.48631365         3.55238806
      4.75128699         8.22947047         3.55238806
      6.33504932         5.48631365         3.55238806
      7.91881165         2.74315682         3.55238806
      9.50257398         0.00000000         3.55238806
     11.08633632        -2.74315682         3.55238806
```

```
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
```

```
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
11.08633632  -0.91438561   1.77619403
12.67009865  -1.82877122   1.77619403
12.67009865  -3.65754243   1.77619403
 7.91881165  11.88701290   1.77619403
 7.91881165  10.05824169   1.77619403
 9.50257398   9.14385608   1.77619403
 9.50257398   7.31508486   1.77619403
```

```
 11.08633632   6.40069926   1.77619403
 11.08633632   4.57192804   1.77619403
 12.67009865   3.65754243   1.77619403
 12.67009865   1.82877122   1.77619403
 14.25386098   0.91438561   1.77619403
 14.25386098  -0.91438561   1.77619403
  1.58376233   0.91438561   5.32858209
  1.58376233  -0.91438561   5.32858209
  3.16752466  -1.82877122   5.32858209
  3.16752466  -3.65754243   5.32858209
  4.75128699  -4.57192804   5.32858209
  4.75128699  -6.40069926   5.32858209
  6.33504932  -7.31508486   5.32858209
  6.33504932  -9.14385608   5.32858209
  7.91881165 -10.05824169   5.32858209
  7.91881165 -11.88701290   5.32858209
  3.16752466   3.65754243   5.32858209
  3.16752466   1.82877122   5.32858209
  4.75128699   0.91438561   5.32858209
  4.75128699  -0.91438561   5.32858209
  6.33504932  -1.82877122   5.32858209
  6.33504932  -3.65754243   5.32858209
  7.91881165  -4.57192804   5.32858209
  7.91881165  -6.40069926   5.32858209
  9.50257398  -7.31508486   5.32858209
  9.50257398  -9.14385608   5.32858209
  4.75128699   6.40069926   5.32858209
  4.75128699   4.57192804   5.32858209
  6.33504932   3.65754243   5.32858209
  6.33504932   1.82877122   5.32858209
  7.91881165   0.91438561   5.32858209
  7.91881165  -0.91438561   5.32858209
  9.50257398  -1.82877122   5.32858209
  9.50257398  -3.65754243   5.32858209
 11.08633632  -4.57192804   5.32858209
 11.08633632  -6.40069926   5.32858209
  6.33504932   9.14385608   5.32858209
  6.33504932   7.31508486   5.32858209
  7.91881165   6.40069926   5.32858209
  7.91881165   4.57192804   5.32858209
  9.50257398   3.65754243   5.32858209
  9.50257398   1.82877122   5.32858209
 11.08633632   0.91438561   5.32858209
 11.08633632  -0.91438561   5.32858209
 12.67009865  -1.82877122   5.32858209
 12.67009865  -3.65754243   5.32858209
  7.91881165  11.88701290   5.32858209
  7.91881165  10.05824169   5.32858209
  9.50257398   9.14385608   5.32858209
  9.50257398   7.31508486   5.32858209
 11.08633632   6.40069926   5.32858209
 11.08633632   4.57192804   5.32858209
 12.67009865   3.65754243   5.32858209
 12.67009865   1.82877122   5.32858209
 14.25386098   0.91438561   5.32858209
 14.25386098  -0.91438561   5.32858209
  1.58376233   0.91438561   8.88097015
  1.58376233  -0.91438561   8.88097015
  3.16752466  -1.82877122   8.88097015
  3.16752466  -3.65754243   8.88097015
  4.75128699  -4.57192804   8.88097015
  4.75128699  -6.40069926   8.88097015
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```
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 6.33504932  -9.14385608   8.88097015
 7.91881165 -10.05824169   8.88097015
 7.91881165 -11.88701290   8.88097015
 3.16752466   3.65754243   8.88097015
 3.16752466   1.82877122   8.88097015
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 4.75128699  -0.91438561   8.88097015
 6.33504932  -1.82877122   8.88097015
 6.33504932  -3.65754243   8.88097015
 7.91881165  -4.57192804   8.88097015
 7.91881165  -6.40069926   8.88097015
 9.50257398  -7.31508486   8.88097015
 9.50257398  -9.14385608   8.88097015
 4.75128699   6.40069926   8.88097015
 4.75128699   4.57192804   8.88097015
 6.33504932   3.65754243   8.88097015
 6.33504932   1.82877122   8.88097015
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 7.91881165  -0.91438561   8.88097015
 9.50257398  -1.82877122   8.88097015
 9.50257398  -3.65754243   8.88097015
11.08633632  -4.57192804   8.88097015
11.08633632  -6.40069926   8.88097015
 6.33504932   9.14385608   8.88097015
 6.33504932   7.31508486   8.88097015
 7.91881165   6.40069926   8.88097015
 7.91881165   4.57192804   8.88097015
 9.50257398   3.65754243   8.88097015
 9.50257398   1.82877122   8.88097015
11.08633632   0.91438561   8.88097015
11.08633632  -0.91438561   8.88097015
12.67009865  -1.82877122   8.88097015
12.67009865  -3.65754243   8.88097015
 7.91881165  11.88701290   8.88097015
 7.91881165  10.05824169   8.88097015
 9.50257398   9.14385608   8.88097015
 9.50257398   7.31508486   8.88097015
11.08633632   6.40069926   8.88097015
11.08633632   4.57192804   8.88097015
12.67009865   3.65754243   8.88097015
12.67009865   1.82877122   8.88097015
14.25386098   0.91438561   8.88097015
14.25386098  -0.91438561   8.88097015
 1.58376233   0.91438561  12.43335821
 1.58376233  -0.91438561  12.43335821
 3.16752466  -1.82877122  12.43335821
 3.16752466  -3.65754243  12.43335821
 4.75128699  -4.57192804  12.43335821
 4.75128699  -6.40069926  12.43335821
 6.33504932  -7.31508486  12.43335821
 6.33504932  -9.14385608  12.43335821
 7.91881165 -10.05824169  12.43335821
 7.91881165 -11.88701290  12.43335821
 3.16752466   3.65754243  12.43335821
 3.16752466   1.82877122  12.43335821
 4.75128699   0.91438561  12.43335821
 4.75128699  -0.91438561  12.43335821
 6.33504932  -1.82877122  12.43335821
 6.33504932  -3.65754243  12.43335821
 7.91881165  -4.57192804  12.43335821
 7.91881165  -6.40069926  12.43335821
```

```
 9.50257398  -7.31508486  12.43335821
 9.50257398  -9.14385608  12.43335821
 4.75128699   6.40069926  12.43335821
 4.75128699   4.57192804  12.43335821
 6.33504932   3.65754243  12.43335821
 6.33504932   1.82877122  12.43335821
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
 9.50257398   1.82877122  12.43335821
11.08633632   0.91438561  12.43335821
11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
12.67009865  -3.65754243  12.43335821
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
 4.75128699  -4.57192804  15.98574627
 4.75128699  -6.40069926  15.98574627
 6.33504932  -7.31508486  15.98574627
 6.33504932  -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466   3.65754243  15.98574627
 3.16752466   1.82877122  15.98574627
 4.75128699   0.91438561  15.98574627
 4.75128699  -0.91438561  15.98574627
 6.33504932  -1.82877122  15.98574627
 6.33504932  -3.65754243  15.98574627
 7.91881165  -4.57192804  15.98574627
 7.91881165  -6.40069926  15.98574627
 9.50257398  -7.31508486  15.98574627
 9.50257398  -9.14385608  15.98574627
 4.75128699   6.40069926  15.98574627
 4.75128699   4.57192804  15.98574627
 6.33504932   3.65754243  15.98574627
 6.33504932   1.82877122  15.98574627
 7.91881165   0.91438561  15.98574627
 7.91881165  -0.91438561  15.98574627
 9.50257398  -1.82877122  15.98574627
 9.50257398  -3.65754243  15.98574627
11.08633632  -4.57192804  15.98574627
11.08633632  -6.40069926  15.98574627
```

```
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   7.91881    0.91439   16.56194
```

Listing 24: Structural input file for configuration: 5x5x5 N B top.

5x5x5_N_B_Zr POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr   B   N
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
      4.75128699         8.22947047         0.00000000
      6.33504932         5.48631365         0.00000000
      7.91881165         2.74315682         0.00000000
      9.50257398         0.00000000         0.00000000
     11.08633632        -2.74315682         0.00000000
      6.33504932        10.97262730         0.00000000
      7.91881165         8.22947047         0.00000000
      9.50257398         5.48631365         0.00000000
     11.08633632         2.74315682         0.00000000
     12.67009865         0.00000000         0.00000000
      0.00000000         0.00000000         3.55238806
      1.58376233        -2.74315682         3.55238806
```

```
 3.16752466  -5.48631365   3.55238806
 4.75128699  -8.22947047   3.55238806
 6.33504932 -10.97262730   3.55238806
 1.58376233   2.74315682   3.55238806
 3.16752466   0.00000000   3.55238806
 4.75128699  -2.74315682   3.55238806
 6.33504932  -5.48631365   3.55238806
 7.91881165  -8.22947047   3.55238806
 3.16752466   5.48631365   3.55238806
 4.75128699   2.74315682   3.55238806
 6.33504932   0.00000000   3.55238806
 7.91881165  -2.74315682   3.55238806
 9.50257398  -5.48631365   3.55238806
 4.75128699   8.22947047   3.55238806
 6.33504932   5.48631365   3.55238806
 7.91881165   2.74315682   3.55238806
 9.50257398   0.00000000   3.55238806
11.08633632  -2.74315682   3.55238806
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
```

```
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
```

```
 9.50257398       -1.82877122        1.77619403
 9.50257398       -3.65754243        1.77619403
11.08633632       -4.57192804        1.77619403
11.08633632       -6.40069926        1.77619403
 6.33504932        9.14385608        1.77619403
 6.33504932        7.31508486        1.77619403
 7.91881165        6.40069926        1.77619403
 7.91881165        4.57192804        1.77619403
 9.50257398        3.65754243        1.77619403
 9.50257398        1.82877122        1.77619403
11.08633632        0.91438561        1.77619403
11.08633632       -0.91438561        1.77619403
12.67009865       -1.82877122        1.77619403
12.67009865       -3.65754243        1.77619403
 7.91881165       11.88701290        1.77619403
 7.91881165       10.05824169        1.77619403
 9.50257398        9.14385608        1.77619403
 9.50257398        7.31508486        1.77619403
11.08633632        6.40069926        1.77619403
11.08633632        4.57192804        1.77619403
12.67009865        3.65754243        1.77619403
12.67009865        1.82877122        1.77619403
14.25386098        0.91438561        1.77619403
14.25386098       -0.91438561        1.77619403
 1.58376233        0.91438561        5.32858209
 1.58376233       -0.91438561        5.32858209
 3.16752466       -1.82877122        5.32858209
 3.16752466       -3.65754243        5.32858209
 4.75128699       -4.57192804        5.32858209
 4.75128699       -6.40069926        5.32858209
 6.33504932       -7.31508486        5.32858209
 6.33504932       -9.14385608        5.32858209
 7.91881165      -10.05824169        5.32858209
 7.91881165      -11.88701290        5.32858209
 3.16752466        3.65754243        5.32858209
 3.16752466        1.82877122        5.32858209
 4.75128699        0.91438561        5.32858209
 4.75128699       -0.91438561        5.32858209
 6.33504932       -1.82877122        5.32858209
 6.33504932       -3.65754243        5.32858209
 7.91881165       -4.57192804        5.32858209
 7.91881165       -6.40069926        5.32858209
 9.50257398       -7.31508486        5.32858209
 9.50257398       -9.14385608        5.32858209
 4.75128699        6.40069926        5.32858209
 4.75128699        4.57192804        5.32858209
 6.33504932        3.65754243        5.32858209
 6.33504932        1.82877122        5.32858209
 7.91881165        0.91438561        5.32858209
 7.91881165       -0.91438561        5.32858209
 9.50257398       -1.82877122        5.32858209
 9.50257398       -3.65754243        5.32858209
11.08633632       -4.57192804        5.32858209
11.08633632       -6.40069926        5.32858209
 6.33504932        9.14385608        5.32858209
 6.33504932        7.31508486        5.32858209
 7.91881165        6.40069926        5.32858209
 7.91881165        4.57192804        5.32858209
 9.50257398        3.65754243        5.32858209
 9.50257398        1.82877122        5.32858209
11.08633632        0.91438561        5.32858209
11.08633632       -0.91438561        5.32858209
```

```
 12.67009865  -1.82877122  5.32858209
 12.67009865  -3.65754243  5.32858209
  7.91881165  11.88701290  5.32858209
  7.91881165  10.05824169  5.32858209
  9.50257398   9.14385608  5.32858209
  9.50257398   7.31508486  5.32858209
 11.08633632   6.40069926  5.32858209
 11.08633632   4.57192804  5.32858209
 12.67009865   3.65754243  5.32858209
 12.67009865   1.82877122  5.32858209
 14.25386098   0.91438561  5.32858209
 14.25386098  -0.91438561  5.32858209
  1.58376233   0.91438561  8.88097015
  1.58376233  -0.91438561  8.88097015
  3.16752466  -1.82877122  8.88097015
  3.16752466  -3.65754243  8.88097015
  4.75128699  -4.57192804  8.88097015
  4.75128699  -6.40069926  8.88097015
  6.33504932  -7.31508486  8.88097015
  6.33504932  -9.14385608  8.88097015
  7.91881165 -10.05824169  8.88097015
  7.91881165 -11.88701290  8.88097015
  3.16752466   3.65754243  8.88097015
  3.16752466   1.82877122  8.88097015
  4.75128699   0.91438561  8.88097015
  4.75128699  -0.91438561  8.88097015
  6.33504932  -1.82877122  8.88097015
  6.33504932  -3.65754243  8.88097015
  7.91881165  -4.57192804  8.88097015
  7.91881165  -6.40069926  8.88097015
  9.50257398  -7.31508486  8.88097015
  9.50257398  -9.14385608  8.88097015
  4.75128699   6.40069926  8.88097015
  4.75128699   4.57192804  8.88097015
  6.33504932   3.65754243  8.88097015
  6.33504932   1.82877122  8.88097015
  7.91881165   0.91438561  8.88097015
  7.91881165  -0.91438561  8.88097015
  9.50257398  -1.82877122  8.88097015
  9.50257398  -3.65754243  8.88097015
 11.08633632  -4.57192804  8.88097015
 11.08633632  -6.40069926  8.88097015
  6.33504932   9.14385608  8.88097015
  6.33504932   7.31508486  8.88097015
  7.91881165   6.40069926  8.88097015
  7.91881165   4.57192804  8.88097015
  9.50257398   3.65754243  8.88097015
  9.50257398   1.82877122  8.88097015
 11.08633632   0.91438561  8.88097015
 11.08633632  -0.91438561  8.88097015
 12.67009865  -1.82877122  8.88097015
 12.67009865  -3.65754243  8.88097015
  7.91881165  11.88701290  8.88097015
  7.91881165  10.05824169  8.88097015
  9.50257398   9.14385608  8.88097015
  9.50257398   7.31508486  8.88097015
 11.08633632   6.40069926  8.88097015
 11.08633632   4.57192804  8.88097015
 12.67009865   3.65754243  8.88097015
 12.67009865   1.82877122  8.88097015
 14.25386098   0.91438561  8.88097015
 14.25386098  -0.91438561  8.88097015
```

```
 1.58376233   0.91438561  12.43335821
 1.58376233  -0.91438561  12.43335821
 3.16752466  -1.82877122  12.43335821
 3.16752466  -3.65754243  12.43335821
 4.75128699  -4.57192804  12.43335821
 4.75128699  -6.40069926  12.43335821
 6.33504932  -7.31508486  12.43335821
 6.33504932  -9.14385608  12.43335821
 7.91881165 -10.05824169  12.43335821
 7.91881165 -11.88701290  12.43335821
 3.16752466   3.65754243  12.43335821
 3.16752466   1.82877122  12.43335821
 4.75128699   0.91438561  12.43335821
 4.75128699  -0.91438561  12.43335821
 6.33504932  -1.82877122  12.43335821
 6.33504932  -3.65754243  12.43335821
 7.91881165  -4.57192804  12.43335821
 7.91881165  -6.40069926  12.43335821
 9.50257398  -7.31508486  12.43335821
 9.50257398  -9.14385608  12.43335821
 4.75128699   6.40069926  12.43335821
 4.75128699   4.57192804  12.43335821
 6.33504932   3.65754243  12.43335821
 6.33504932   1.82877122  12.43335821
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
 9.50257398   1.82877122  12.43335821
11.08633632   0.91438561  12.43335821
11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
12.67009865  -3.65754243  12.43335821
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
 4.75128699  -4.57192804  15.98574627
 4.75128699  -6.40069926  15.98574627
 6.33504932  -7.31508486  15.98574627
 6.33504932  -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466   3.65754243  15.98574627
 3.16752466   1.82877122  15.98574627
```

```
      4.75128699         0.91438561        15.98574627
      4.75128699        -0.91438561        15.98574627
      6.33504932        -1.82877122        15.98574627
      6.33504932        -3.65754243        15.98574627
      7.91881165        -4.57192804        15.98574627
      7.91881165        -6.40069926        15.98574627
      9.50257398        -7.31508486        15.98574627
      9.50257398        -9.14385608        15.98574627
      4.75128699         6.40069926        15.98574627
      4.75128699         4.57192804        15.98574627
      6.33504932         3.65754243        15.98574627
      6.33504932         1.82877122        15.98574627
      7.91881165         0.91438561        15.98574627
      7.91881165        -0.91438561        15.98574627
      9.50257398        -1.82877122        15.98574627
      9.50257398        -3.65754243        15.98574627
     11.08633632        -4.57192804        15.98574627
     11.08633632        -6.40069926        15.98574627
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   7.91881   1.8439  16.8194
```

Listing 25: Structural input file for configuration: 5x5x5 N B Zr.

5x5x5_N_Zr_ring POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr  B  N
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
```

```
 7.91881165  -8.22947047  0.00000000
 3.16752466   5.48631365  0.00000000
 4.75128699   2.74315682  0.00000000
 6.33504932   0.00000000  0.00000000
 7.91881165  -2.74315682  0.00000000
 9.50257398  -5.48631365  0.00000000
 4.75128699   8.22947047  0.00000000
 6.33504932   5.48631365  0.00000000
 7.91881165   2.74315682  0.00000000
 9.50257398   0.00000000  0.00000000
11.08633632  -2.74315682  0.00000000
 6.33504932  10.97262730  0.00000000
 7.91881165   8.22947047  0.00000000
 9.50257398   5.48631365  0.00000000
11.08633632   2.74315682  0.00000000
12.67009865   0.00000000  0.00000000
 0.00000000   0.00000000  3.55238806
 1.58376233  -2.74315682  3.55238806
 3.16752466  -5.48631365  3.55238806
 4.75128699  -8.22947047  3.55238806
 6.33504932 -10.97262730  3.55238806
 1.58376233   2.74315682  3.55238806
 3.16752466   0.00000000  3.55238806
 4.75128699  -2.74315682  3.55238806
 6.33504932  -5.48631365  3.55238806
 7.91881165  -8.22947047  3.55238806
 3.16752466   5.48631365  3.55238806
 4.75128699   2.74315682  3.55238806
 6.33504932   0.00000000  3.55238806
 7.91881165  -2.74315682  3.55238806
 9.50257398  -5.48631365  3.55238806
 4.75128699   8.22947047  3.55238806
 6.33504932   5.48631365  3.55238806
 7.91881165   2.74315682  3.55238806
 9.50257398   0.00000000  3.55238806
11.08633632  -2.74315682  3.55238806
 6.33504932  10.97262730  3.55238806
 7.91881165   8.22947047  3.55238806
 9.50257398   5.48631365  3.55238806
11.08633632   2.74315682  3.55238806
12.67009865   0.00000000  3.55238806
 0.00000000   0.00000000  7.10477612
 1.58376233  -2.74315682  7.10477612
 3.16752466  -5.48631365  7.10477612
 4.75128699  -8.22947047  7.10477612
 6.33504932 -10.97262730  7.10477612
 1.58376233   2.74315682  7.10477612
 3.16752466   0.00000000  7.10477612
 4.75128699  -2.74315682  7.10477612
 6.33504932  -5.48631365  7.10477612
 7.91881165  -8.22947047  7.10477612
 3.16752466   5.48631365  7.10477612
 4.75128699   2.74315682  7.10477612
 6.33504932   0.00000000  7.10477612
 7.91881165  -2.74315682  7.10477612
 9.50257398  -5.48631365  7.10477612
 4.75128699   8.22947047  7.10477612
 6.33504932   5.48631365  7.10477612
 7.91881165   2.74315682  7.10477612
 9.50257398   0.00000000  7.10477612
11.08633632  -2.74315682  7.10477612
 6.33504932  10.97262730  7.10477612
```

```
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
```

```
 7.91881165      -10.05824169        1.77619403
 7.91881165      -11.88701290        1.77619403
 3.16752466        3.65754243        1.77619403
 3.16752466        1.82877122        1.77619403
 4.75128699        0.91438561        1.77619403
 4.75128699       -0.91438561        1.77619403
 6.33504932       -1.82877122        1.77619403
 6.33504932       -3.65754243        1.77619403
 7.91881165       -4.57192804        1.77619403
 7.91881165       -6.40069926        1.77619403
 9.50257398       -7.31508486        1.77619403
 9.50257398       -9.14385608        1.77619403
 4.75128699        6.40069926        1.77619403
 4.75128699        4.57192804        1.77619403
 6.33504932        3.65754243        1.77619403
 6.33504932        1.82877122        1.77619403
 7.91881165        0.91438561        1.77619403
 7.91881165       -0.91438561        1.77619403
 9.50257398       -1.82877122        1.77619403
 9.50257398       -3.65754243        1.77619403
11.08633632       -4.57192804        1.77619403
11.08633632       -6.40069926        1.77619403
 6.33504932        9.14385608        1.77619403
 6.33504932        7.31508486        1.77619403
 7.91881165        6.40069926        1.77619403
 7.91881165        4.57192804        1.77619403
 9.50257398        3.65754243        1.77619403
 9.50257398        1.82877122        1.77619403
11.08633632        0.91438561        1.77619403
11.08633632       -0.91438561        1.77619403
12.67009865       -1.82877122        1.77619403
12.67009865       -3.65754243        1.77619403
 7.91881165       11.88701290        1.77619403
 7.91881165       10.05824169        1.77619403
 9.50257398        9.14385608        1.77619403
 9.50257398        7.31508486        1.77619403
11.08633632        6.40069926        1.77619403
11.08633632        4.57192804        1.77619403
12.67009865        3.65754243        1.77619403
12.67009865        1.82877122        1.77619403
14.25386098        0.91438561        1.77619403
14.25386098       -0.91438561        1.77619403
 1.58376233        0.91438561        5.32858209
 1.58376233       -0.91438561        5.32858209
 3.16752466       -1.82877122        5.32858209
 3.16752466       -3.65754243        5.32858209
 4.75128699       -4.57192804        5.32858209
 4.75128699       -6.40069926        5.32858209
 6.33504932       -7.31508486        5.32858209
 6.33504932       -9.14385608        5.32858209
 7.91881165      -10.05824169        5.32858209
 7.91881165      -11.88701290        5.32858209
 3.16752466        3.65754243        5.32858209
 3.16752466        1.82877122        5.32858209
 4.75128699        0.91438561        5.32858209
 4.75128699       -0.91438561        5.32858209
 6.33504932       -1.82877122        5.32858209
 6.33504932       -3.65754243        5.32858209
 7.91881165       -4.57192804        5.32858209
 7.91881165       -6.40069926        5.32858209
 9.50257398       -7.31508486        5.32858209
 9.50257398       -9.14385608        5.32858209
```

```
 4.75128699  6.40069926  5.32858209
 4.75128699  4.57192804  5.32858209
 6.33504932  3.65754243  5.32858209
 6.33504932  1.82877122  5.32858209
 7.91881165  0.91438561  5.32858209
 7.91881165 -0.91438561  5.32858209
 9.50257398 -1.82877122  5.32858209
 9.50257398 -3.65754243  5.32858209
11.08633632 -4.57192804  5.32858209
11.08633632 -6.40069926  5.32858209
 6.33504932  9.14385608  5.32858209
 6.33504932  7.31508486  5.32858209
 7.91881165  6.40069926  5.32858209
 7.91881165  4.57192804  5.32858209
 9.50257398  3.65754243  5.32858209
 9.50257398  1.82877122  5.32858209
11.08633632  0.91438561  5.32858209
11.08633632 -0.91438561  5.32858209
12.67009865 -1.82877122  5.32858209
12.67009865 -3.65754243  5.32858209
 7.91881165 11.88701290  5.32858209
 7.91881165 10.05824169  5.32858209
 9.50257398  9.14385608  5.32858209
 9.50257398  7.31508486  5.32858209
11.08633632  6.40069926  5.32858209
11.08633632  4.57192804  5.32858209
12.67009865  3.65754243  5.32858209
12.67009865  1.82877122  5.32858209
14.25386098  0.91438561  5.32858209
14.25386098 -0.91438561  5.32858209
 1.58376233  0.91438561  8.88097015
 1.58376233 -0.91438561  8.88097015
 3.16752466 -1.82877122  8.88097015
 3.16752466 -3.65754243  8.88097015
 4.75128699 -4.57192804  8.88097015
 4.75128699 -6.40069926  8.88097015
 6.33504932 -7.31508486  8.88097015
 6.33504932 -9.14385608  8.88097015
 7.91881165 -10.05824169  8.88097015
 7.91881165 -11.88701290  8.88097015
 3.16752466  3.65754243  8.88097015
 3.16752466  1.82877122  8.88097015
 4.75128699  0.91438561  8.88097015
 4.75128699 -0.91438561  8.88097015
 6.33504932 -1.82877122  8.88097015
 6.33504932 -3.65754243  8.88097015
 7.91881165 -4.57192804  8.88097015
 7.91881165 -6.40069926  8.88097015
 9.50257398 -7.31508486  8.88097015
 9.50257398 -9.14385608  8.88097015
 4.75128699  6.40069926  8.88097015
 4.75128699  4.57192804  8.88097015
 6.33504932  3.65754243  8.88097015
 6.33504932  1.82877122  8.88097015
 7.91881165  0.91438561  8.88097015
 7.91881165 -0.91438561  8.88097015
 9.50257398 -1.82877122  8.88097015
 9.50257398 -3.65754243  8.88097015
11.08633632 -4.57192804  8.88097015
11.08633632 -6.40069926  8.88097015
 6.33504932  9.14385608  8.88097015
 6.33504932  7.31508486  8.88097015
```

```
 7.91881165  6.40069926  8.88097015
 7.91881165  4.57192804  8.88097015
 9.50257398  3.65754243  8.88097015
 9.50257398  1.82877122  8.88097015
11.08633632  0.91438561  8.88097015
11.08633632 -0.91438561  8.88097015
12.67009865 -1.82877122  8.88097015
12.67009865 -3.65754243  8.88097015
 7.91881165 11.88701290  8.88097015
 7.91881165 10.05824169  8.88097015
 9.50257398  9.14385608  8.88097015
 9.50257398  7.31508486  8.88097015
11.08633632  6.40069926  8.88097015
11.08633632  4.57192804  8.88097015
12.67009865  3.65754243  8.88097015
12.67009865  1.82877122  8.88097015
14.25386098  0.91438561  8.88097015
14.25386098 -0.91438561  8.88097015
 1.58376233  0.91438561 12.43335821
 1.58376233 -0.91438561 12.43335821
 3.16752466 -1.82877122 12.43335821
 3.16752466 -3.65754243 12.43335821
 4.75128699 -4.57192804 12.43335821
 4.75128699 -6.40069926 12.43335821
 6.33504932 -7.31508486 12.43335821
 6.33504932 -9.14385608 12.43335821
 7.91881165 -10.05824169 12.43335821
 7.91881165 -11.88701290 12.43335821
 3.16752466  3.65754243 12.43335821
 3.16752466  1.82877122 12.43335821
 4.75128699  0.91438561 12.43335821
 4.75128699 -0.91438561 12.43335821
 6.33504932 -1.82877122 12.43335821
 6.33504932 -3.65754243 12.43335821
 7.91881165 -4.57192804 12.43335821
 7.91881165 -6.40069926 12.43335821
 9.50257398 -7.31508486 12.43335821
 9.50257398 -9.14385608 12.43335821
 4.75128699  6.40069926 12.43335821
 4.75128699  4.57192804 12.43335821
 6.33504932  3.65754243 12.43335821
 6.33504932  1.82877122 12.43335821
 7.91881165  0.91438561 12.43335821
 7.91881165 -0.91438561 12.43335821
 9.50257398 -1.82877122 12.43335821
 9.50257398 -3.65754243 12.43335821
11.08633632 -4.57192804 12.43335821
11.08633632 -6.40069926 12.43335821
 6.33504932  9.14385608 12.43335821
 6.33504932  7.31508486 12.43335821
 7.91881165  6.40069926 12.43335821
 7.91881165  4.57192804 12.43335821
 9.50257398  3.65754243 12.43335821
 9.50257398  1.82877122 12.43335821
11.08633632  0.91438561 12.43335821
11.08633632 -0.91438561 12.43335821
12.67009865 -1.82877122 12.43335821
12.67009865 -3.65754243 12.43335821
 7.91881165 11.88701290 12.43335821
 7.91881165 10.05824169 12.43335821
 9.50257398  9.14385608 12.43335821
 9.50257398  7.31508486 12.43335821
```

```
    11.08633632         6.40069926        12.43335821
    11.08633632         4.57192804        12.43335821
    12.67009865         3.65754243        12.43335821
    12.67009865         1.82877122        12.43335821
    14.25386098         0.91438561        12.43335821
    14.25386098        -0.91438561        12.43335821
     1.58376233         0.91438561        15.98574627
     1.58376233        -0.91438561        15.98574627
     3.16752466        -1.82877122        15.98574627
     3.16752466        -3.65754243        15.98574627
     4.75128699        -4.57192804        15.98574627
     4.75128699        -6.40069926        15.98574627
     6.33504932        -7.31508486        15.98574627
     6.33504932        -9.14385608        15.98574627
     7.91881165       -10.05824169        15.98574627
     7.91881165       -11.88701290        15.98574627
     3.16752466         3.65754243        15.98574627
     3.16752466         1.82877122        15.98574627
     4.75128699         0.91438561        15.98574627
     4.75128699        -0.91438561        15.98574627
     6.33504932        -1.82877122        15.98574627
     6.33504932        -3.65754243        15.98574627
     7.91881165        -4.57192804        15.98574627
     7.91881165        -6.40069926        15.98574627
     9.50257398        -7.31508486        15.98574627
     9.50257398        -9.14385608        15.98574627
     4.75128699         6.40069926        15.98574627
     4.75128699         4.57192804        15.98574627
     6.33504932         3.65754243        15.98574627
     6.33504932         1.82877122        15.98574627
     7.91881165         0.91438561        15.98574627
     7.91881165        -0.91438561        15.98574627
     9.50257398        -1.82877122        15.98574627
     9.50257398        -3.65754243        15.98574627
    11.08633632        -4.57192804        15.98574627
    11.08633632        -6.40069926        15.98574627
     6.33504932         9.14385608        15.98574627
     6.33504932         7.31508486        15.98574627
     7.91881165         6.40069926        15.98574627
     7.91881165         4.57192804        15.98574627
     9.50257398         3.65754243        15.98574627
     9.50257398         1.82877122        15.98574627
    11.08633632         0.91438561        15.98574627
    11.08633632        -0.91438561        15.98574627
    12.67009865        -1.82877122        15.98574627
    12.67009865        -3.65754243        15.98574627
     7.91881165        11.88701290        15.98574627
     7.91881165        10.05824169        15.98574627
     9.50257398         9.14385608        15.98574627
     9.50257398         7.31508486        15.98574627
    11.08633632         6.40069926        15.98574627
    11.08633632         4.57192804        15.98574627
    12.67009865         3.65754243        15.98574627
    12.67009865         1.82877122        15.98574627
    14.25386098         0.91438561        15.98574627
    14.25386098        -0.91438561        15.98574627
  7.91881   0.91439  17.76194
```

Listing 26: Structural input file for configuration: 5x5x5 N Zr ring.

5x5x5_O_B_top POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr   B   O
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
      4.75128699         8.22947047         0.00000000
      6.33504932         5.48631365         0.00000000
      7.91881165         2.74315682         0.00000000
      9.50257398         0.00000000         0.00000000
     11.08633632        -2.74315682         0.00000000
      6.33504932        10.97262730         0.00000000
      7.91881165         8.22947047         0.00000000
      9.50257398         5.48631365         0.00000000
     11.08633632         2.74315682         0.00000000
     12.67009865         0.00000000         0.00000000
      0.00000000         0.00000000         3.55238806
      1.58376233        -2.74315682         3.55238806
      3.16752466        -5.48631365         3.55238806
      4.75128699        -8.22947047         3.55238806
      6.33504932       -10.97262730         3.55238806
      1.58376233         2.74315682         3.55238806
      3.16752466         0.00000000         3.55238806
      4.75128699        -2.74315682         3.55238806
      6.33504932        -5.48631365         3.55238806
      7.91881165        -8.22947047         3.55238806
      3.16752466         5.48631365         3.55238806
      4.75128699         2.74315682         3.55238806
      6.33504932         0.00000000         3.55238806
      7.91881165        -2.74315682         3.55238806
      9.50257398        -5.48631365         3.55238806
      4.75128699         8.22947047         3.55238806
      6.33504932         5.48631365         3.55238806
      7.91881165         2.74315682         3.55238806
      9.50257398         0.00000000         3.55238806
     11.08633632        -2.74315682         3.55238806
      6.33504932        10.97262730         3.55238806
      7.91881165         8.22947047         3.55238806
      9.50257398         5.48631365         3.55238806
     11.08633632         2.74315682         3.55238806
     12.67009865         0.00000000         3.55238806
      0.00000000         0.00000000         7.10477612
```

```
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
```

```
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
11.08633632  -0.91438561   1.77619403
12.67009865  -1.82877122   1.77619403
12.67009865  -3.65754243   1.77619403
 7.91881165  11.88701290   1.77619403
 7.91881165  10.05824169   1.77619403
 9.50257398   9.14385608   1.77619403
 9.50257398   7.31508486   1.77619403
11.08633632   6.40069926   1.77619403
11.08633632   4.57192804   1.77619403
12.67009865   3.65754243   1.77619403
12.67009865   1.82877122   1.77619403
14.25386098   0.91438561   1.77619403
14.25386098  -0.91438561   1.77619403
```

```
 1.58376233   0.91438561   5.32858209
 1.58376233  -0.91438561   5.32858209
 3.16752466  -1.82877122   5.32858209
 3.16752466  -3.65754243   5.32858209
 4.75128699  -4.57192804   5.32858209
 4.75128699  -6.40069926   5.32858209
 6.33504932  -7.31508486   5.32858209
 6.33504932  -9.14385608   5.32858209
 7.91881165 -10.05824169   5.32858209
 7.91881165 -11.88701290   5.32858209
 3.16752466   3.65754243   5.32858209
 3.16752466   1.82877122   5.32858209
 4.75128699   0.91438561   5.32858209
 4.75128699  -0.91438561   5.32858209
 6.33504932  -1.82877122   5.32858209
 6.33504932  -3.65754243   5.32858209
 7.91881165  -4.57192804   5.32858209
 7.91881165  -6.40069926   5.32858209
 9.50257398  -7.31508486   5.32858209
 9.50257398  -9.14385608   5.32858209
 4.75128699   6.40069926   5.32858209
 4.75128699   4.57192804   5.32858209
 6.33504932   3.65754243   5.32858209
 6.33504932   1.82877122   5.32858209
 7.91881165   0.91438561   5.32858209
 7.91881165  -0.91438561   5.32858209
 9.50257398  -1.82877122   5.32858209
 9.50257398  -3.65754243   5.32858209
11.08633632  -4.57192804   5.32858209
11.08633632  -6.40069926   5.32858209
 6.33504932   9.14385608   5.32858209
 6.33504932   7.31508486   5.32858209
 7.91881165   6.40069926   5.32858209
 7.91881165   4.57192804   5.32858209
 9.50257398   3.65754243   5.32858209
 9.50257398   1.82877122   5.32858209
11.08633632   0.91438561   5.32858209
11.08633632  -0.91438561   5.32858209
12.67009865  -1.82877122   5.32858209
12.67009865  -3.65754243   5.32858209
 7.91881165  11.88701290   5.32858209
 7.91881165  10.05824169   5.32858209
 9.50257398   9.14385608   5.32858209
 9.50257398   7.31508486   5.32858209
11.08633632   6.40069926   5.32858209
11.08633632   4.57192804   5.32858209
12.67009865   3.65754243   5.32858209
12.67009865   1.82877122   5.32858209
14.25386098   0.91438561   5.32858209
14.25386098  -0.91438561   5.32858209
 1.58376233   0.91438561   8.88097015
 1.58376233  -0.91438561   8.88097015
 3.16752466  -1.82877122   8.88097015
 3.16752466  -3.65754243   8.88097015
 4.75128699  -4.57192804   8.88097015
 4.75128699  -6.40069926   8.88097015
 6.33504932  -7.31508486   8.88097015
 6.33504932  -9.14385608   8.88097015
 7.91881165 -10.05824169   8.88097015
 7.91881165 -11.88701290   8.88097015
 3.16752466   3.65754243   8.88097015
 3.16752466   1.82877122   8.88097015
```

```
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 4.75128699 -0.91438561  8.88097015
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 6.33504932 -3.65754243  8.88097015
 7.91881165 -4.57192804  8.88097015
 7.91881165 -6.40069926  8.88097015
 9.50257398 -7.31508486  8.88097015
 9.50257398 -9.14385608  8.88097015
 4.75128699  6.40069926  8.88097015
 4.75128699  4.57192804  8.88097015
 6.33504932  3.65754243  8.88097015
 6.33504932  1.82877122  8.88097015
 7.91881165  0.91438561  8.88097015
 7.91881165 -0.91438561  8.88097015
 9.50257398 -1.82877122  8.88097015
 9.50257398 -3.65754243  8.88097015
11.08633632 -4.57192804  8.88097015
11.08633632 -6.40069926  8.88097015
 6.33504932  9.14385608  8.88097015
 6.33504932  7.31508486  8.88097015
 7.91881165  6.40069926  8.88097015
 7.91881165  4.57192804  8.88097015
 9.50257398  3.65754243  8.88097015
 9.50257398  1.82877122  8.88097015
11.08633632  0.91438561  8.88097015
11.08633632 -0.91438561  8.88097015
12.67009865 -1.82877122  8.88097015
12.67009865 -3.65754243  8.88097015
 7.91881165 11.88701290  8.88097015
 7.91881165 10.05824169  8.88097015
 9.50257398  9.14385608  8.88097015
 9.50257398  7.31508486  8.88097015
11.08633632  6.40069926  8.88097015
11.08633632  4.57192804  8.88097015
12.67009865  3.65754243  8.88097015
12.67009865  1.82877122  8.88097015
14.25386098  0.91438561  8.88097015
14.25386098 -0.91438561  8.88097015
 1.58376233  0.91438561 12.43335821
 1.58376233 -0.91438561 12.43335821
 3.16752466 -1.82877122 12.43335821
 3.16752466 -3.65754243 12.43335821
 4.75128699 -4.57192804 12.43335821
 4.75128699 -6.40069926 12.43335821
 6.33504932 -7.31508486 12.43335821
 6.33504932 -9.14385608 12.43335821
 7.91881165 -10.05824169 12.43335821
 7.91881165 -11.88701290 12.43335821
 3.16752466  3.65754243 12.43335821
 3.16752466  1.82877122 12.43335821
 4.75128699  0.91438561 12.43335821
 4.75128699 -0.91438561 12.43335821
 6.33504932 -1.82877122 12.43335821
 6.33504932 -3.65754243 12.43335821
 7.91881165 -4.57192804 12.43335821
 7.91881165 -6.40069926 12.43335821
 9.50257398 -7.31508486 12.43335821
 9.50257398 -9.14385608 12.43335821
 4.75128699  6.40069926 12.43335821
 4.75128699  4.57192804 12.43335821
 6.33504932  3.65754243 12.43335821
 6.33504932  1.82877122 12.43335821
```

```
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
 9.50257398   1.82877122  12.43335821
11.08633632   0.91438561  12.43335821
11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
12.67009865  -3.65754243  12.43335821
 7.91881165  11.88701290  12.43335821
 7.91881165  10.05824169  12.43335821
 9.50257398   9.14385608  12.43335821
 9.50257398   7.31508486  12.43335821
11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
 4.75128699  -4.57192804  15.98574627
 4.75128699  -6.40069926  15.98574627
 6.33504932  -7.31508486  15.98574627
 6.33504932  -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466   3.65754243  15.98574627
 3.16752466   1.82877122  15.98574627
 4.75128699   0.91438561  15.98574627
 4.75128699  -0.91438561  15.98574627
 6.33504932  -1.82877122  15.98574627
 6.33504932  -3.65754243  15.98574627
 7.91881165  -4.57192804  15.98574627
 7.91881165  -6.40069926  15.98574627
 9.50257398  -7.31508486  15.98574627
 9.50257398  -9.14385608  15.98574627
 4.75128699   6.40069926  15.98574627
 4.75128699   4.57192804  15.98574627
 6.33504932   3.65754243  15.98574627
 6.33504932   1.82877122  15.98574627
 7.91881165   0.91438561  15.98574627
 7.91881165  -0.91438561  15.98574627
 9.50257398  -1.82877122  15.98574627
 9.50257398  -3.65754243  15.98574627
11.08633632  -4.57192804  15.98574627
11.08633632  -6.40069926  15.98574627
 6.33504932   9.14385608  15.98574627
 6.33504932   7.31508486  15.98574627
 7.91881165   6.40069926  15.98574627
 7.91881165   4.57192804  15.98574627
 9.50257398   3.65754243  15.98574627
 9.50257398   1.82877122  15.98574627
```

```
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   7.91881   0.91439  16.56194
```

Listing 27: Structural input file for configuration: 5x5x5 O B top.

5x5x5_O_B_Zr POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr  B  O
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
      4.75128699         8.22947047         0.00000000
      6.33504932         5.48631365         0.00000000
      7.91881165         2.74315682         0.00000000
      9.50257398         0.00000000         0.00000000
     11.08633632        -2.74315682         0.00000000
      6.33504932        10.97262730         0.00000000
      7.91881165         8.22947047         0.00000000
      9.50257398         5.48631365         0.00000000
     11.08633632         2.74315682         0.00000000
     12.67009865         0.00000000         0.00000000
      0.00000000         0.00000000         3.55238806
      1.58376233        -2.74315682         3.55238806
      3.16752466        -5.48631365         3.55238806
      4.75128699        -8.22947047         3.55238806
      6.33504932       -10.97262730         3.55238806
      1.58376233         2.74315682         3.55238806
      3.16752466         0.00000000         3.55238806
      4.75128699        -2.74315682         3.55238806
```

```
 6.33504932  -5.48631365   3.55238806
 7.91881165  -8.22947047   3.55238806
 3.16752466   5.48631365   3.55238806
 4.75128699   2.74315682   3.55238806
 6.33504932   0.00000000   3.55238806
 7.91881165  -2.74315682   3.55238806
 9.50257398  -5.48631365   3.55238806
 4.75128699   8.22947047   3.55238806
 6.33504932   5.48631365   3.55238806
 7.91881165   2.74315682   3.55238806
 9.50257398   0.00000000   3.55238806
11.08633632  -2.74315682   3.55238806
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
```

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 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
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 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
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```
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11.08633632 -0.91438561  1.77619403
12.67009865 -1.82877122  1.77619403
12.67009865 -3.65754243  1.77619403
 7.91881165 11.88701290  1.77619403
 7.91881165 10.05824169  1.77619403
 9.50257398  9.14385608  1.77619403
 9.50257398  7.31508486  1.77619403
11.08633632  6.40069926  1.77619403
11.08633632  4.57192804  1.77619403
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12.67009865  1.82877122  1.77619403
14.25386098  0.91438561  1.77619403
14.25386098 -0.91438561  1.77619403
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 1.58376233 -0.91438561  5.32858209
 3.16752466 -1.82877122  5.32858209
 3.16752466 -3.65754243  5.32858209
 4.75128699 -4.57192804  5.32858209
 4.75128699 -6.40069926  5.32858209
 6.33504932 -7.31508486  5.32858209
 6.33504932 -9.14385608  5.32858209
 7.91881165 -10.05824169 5.32858209
 7.91881165 -11.88701290 5.32858209
 3.16752466  3.65754243  5.32858209
 3.16752466  1.82877122  5.32858209
 4.75128699  0.91438561  5.32858209
 4.75128699 -0.91438561  5.32858209
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 6.33504932 -3.65754243  5.32858209
 7.91881165 -4.57192804  5.32858209
 7.91881165 -6.40069926  5.32858209
 9.50257398 -7.31508486  5.32858209
 9.50257398 -9.14385608  5.32858209
 4.75128699  6.40069926  5.32858209
 4.75128699  4.57192804  5.32858209
 6.33504932  3.65754243  5.32858209
 6.33504932  1.82877122  5.32858209
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 7.91881165 -0.91438561  5.32858209
 9.50257398 -1.82877122  5.32858209
 9.50257398 -3.65754243  5.32858209
11.08633632 -4.57192804  5.32858209
11.08633632 -6.40069926  5.32858209
 6.33504932  9.14385608  5.32858209
 6.33504932  7.31508486  5.32858209
 7.91881165  6.40069926  5.32858209
 7.91881165  4.57192804  5.32858209
 9.50257398  3.65754243  5.32858209
 9.50257398  1.82877122  5.32858209
11.08633632  0.91438561  5.32858209
11.08633632 -0.91438561  5.32858209
12.67009865 -1.82877122  5.32858209
12.67009865 -3.65754243  5.32858209
 7.91881165 11.88701290  5.32858209
 7.91881165 10.05824169  5.32858209
 9.50257398  9.14385608  5.32858209
 9.50257398  7.31508486  5.32858209
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```
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 11.08633632   4.57192804   5.32858209
 12.67009865   3.65754243   5.32858209
 12.67009865   1.82877122   5.32858209
 14.25386098   0.91438561   5.32858209
 14.25386098  -0.91438561   5.32858209
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  1.58376233  -0.91438561   8.88097015
  3.16752466  -1.82877122   8.88097015
  3.16752466  -3.65754243   8.88097015
  4.75128699  -4.57192804   8.88097015
  4.75128699  -6.40069926   8.88097015
  6.33504932  -7.31508486   8.88097015
  6.33504932  -9.14385608   8.88097015
  7.91881165 -10.05824169   8.88097015
  7.91881165 -11.88701290   8.88097015
  3.16752466   3.65754243   8.88097015
  3.16752466   1.82877122   8.88097015
  4.75128699   0.91438561   8.88097015
  4.75128699  -0.91438561   8.88097015
  6.33504932  -1.82877122   8.88097015
  6.33504932  -3.65754243   8.88097015
  7.91881165  -4.57192804   8.88097015
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  9.50257398  -7.31508486   8.88097015
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  4.75128699   4.57192804   8.88097015
  6.33504932   3.65754243   8.88097015
  6.33504932   1.82877122   8.88097015
  7.91881165   0.91438561   8.88097015
  7.91881165  -0.91438561   8.88097015
  9.50257398  -1.82877122   8.88097015
  9.50257398  -3.65754243   8.88097015
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 11.08633632  -6.40069926   8.88097015
  6.33504932   9.14385608   8.88097015
  6.33504932   7.31508486   8.88097015
  7.91881165   6.40069926   8.88097015
  7.91881165   4.57192804   8.88097015
  9.50257398   3.65754243   8.88097015
  9.50257398   1.82877122   8.88097015
 11.08633632   0.91438561   8.88097015
 11.08633632  -0.91438561   8.88097015
 12.67009865  -1.82877122   8.88097015
 12.67009865  -3.65754243   8.88097015
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 11.08633632   6.40069926   8.88097015
 11.08633632   4.57192804   8.88097015
 12.67009865   3.65754243   8.88097015
 12.67009865   1.82877122   8.88097015
 14.25386098   0.91438561   8.88097015
 14.25386098  -0.91438561   8.88097015
  1.58376233   0.91438561  12.43335821
  1.58376233  -0.91438561  12.43335821
  3.16752466  -1.82877122  12.43335821
  3.16752466  -3.65754243  12.43335821
  4.75128699  -4.57192804  12.43335821
  4.75128699  -6.40069926  12.43335821
```

```
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 6.33504932  -9.14385608  12.43335821
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 7.91881165 -11.88701290  12.43335821
 3.16752466   3.65754243  12.43335821
 3.16752466   1.82877122  12.43335821
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 4.75128699  -0.91438561  12.43335821
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 6.33504932  -3.65754243  12.43335821
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 7.91881165  -6.40069926  12.43335821
 9.50257398  -7.31508486  12.43335821
 9.50257398  -9.14385608  12.43335821
 4.75128699   6.40069926  12.43335821
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 9.50257398  -1.82877122  12.43335821
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11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
 7.91881165   6.40069926  12.43335821
 7.91881165   4.57192804  12.43335821
 9.50257398   3.65754243  12.43335821
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11.08633632  -0.91438561  12.43335821
12.67009865  -1.82877122  12.43335821
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 9.50257398   9.14385608  12.43335821
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11.08633632   6.40069926  12.43335821
11.08633632   4.57192804  12.43335821
12.67009865   3.65754243  12.43335821
12.67009865   1.82877122  12.43335821
14.25386098   0.91438561  12.43335821
14.25386098  -0.91438561  12.43335821
 1.58376233   0.91438561  15.98574627
 1.58376233  -0.91438561  15.98574627
 3.16752466  -1.82877122  15.98574627
 3.16752466  -3.65754243  15.98574627
 4.75128699  -4.57192804  15.98574627
 4.75128699  -6.40069926  15.98574627
 6.33504932  -7.31508486  15.98574627
 6.33504932  -9.14385608  15.98574627
 7.91881165 -10.05824169  15.98574627
 7.91881165 -11.88701290  15.98574627
 3.16752466   3.65754243  15.98574627
 3.16752466   1.82877122  15.98574627
 4.75128699   0.91438561  15.98574627
 4.75128699  -0.91438561  15.98574627
 6.33504932  -1.82877122  15.98574627
 6.33504932  -3.65754243  15.98574627
 7.91881165  -4.57192804  15.98574627
 7.91881165  -6.40069926  15.98574627
```

```
      9.50257398        -7.31508486        15.98574627
      9.50257398        -9.14385608        15.98574627
      4.75128699         6.40069926        15.98574627
      4.75128699         4.57192804        15.98574627
      6.33504932         3.65754243        15.98574627
      6.33504932         1.82877122        15.98574627
      7.91881165         0.91438561        15.98574627
      7.91881165        -0.91438561        15.98574627
      9.50257398        -1.82877122        15.98574627
      9.50257398        -3.65754243        15.98574627
     11.08633632        -4.57192804        15.98574627
     11.08633632        -6.40069926        15.98574627
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   7.91881   1.8439  16.8194
```

Listing 28: Structural input file for configuration: 5x5x5 O B Zr.

5x5x5_O_Zr_ring POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
 Zr  B  O
   125     250     1
Cartesian
      0.00000000         0.00000000         0.00000000
      1.58376233        -2.74315682         0.00000000
      3.16752466        -5.48631365         0.00000000
      4.75128699        -8.22947047         0.00000000
      6.33504932       -10.97262730         0.00000000
      1.58376233         2.74315682         0.00000000
      3.16752466         0.00000000         0.00000000
      4.75128699        -2.74315682         0.00000000
      6.33504932        -5.48631365         0.00000000
      7.91881165        -8.22947047         0.00000000
      3.16752466         5.48631365         0.00000000
      4.75128699         2.74315682         0.00000000
      6.33504932         0.00000000         0.00000000
      7.91881165        -2.74315682         0.00000000
      9.50257398        -5.48631365         0.00000000
```

```
 4.75128699   8.22947047   0.00000000
 6.33504932   5.48631365   0.00000000
 7.91881165   2.74315682   0.00000000
 9.50257398   0.00000000   0.00000000
11.08633632  -2.74315682   0.00000000
 6.33504932  10.97262730   0.00000000
 7.91881165   8.22947047   0.00000000
 9.50257398   5.48631365   0.00000000
11.08633632   2.74315682   0.00000000
12.67009865   0.00000000   0.00000000
 0.00000000   0.00000000   3.55238806
 1.58376233  -2.74315682   3.55238806
 3.16752466  -5.48631365   3.55238806
 4.75128699  -8.22947047   3.55238806
 6.33504932 -10.97262730   3.55238806
 1.58376233   2.74315682   3.55238806
 3.16752466   0.00000000   3.55238806
 4.75128699  -2.74315682   3.55238806
 6.33504932  -5.48631365   3.55238806
 7.91881165  -8.22947047   3.55238806
 3.16752466   5.48631365   3.55238806
 4.75128699   2.74315682   3.55238806
 6.33504932   0.00000000   3.55238806
 7.91881165  -2.74315682   3.55238806
 9.50257398  -5.48631365   3.55238806
 4.75128699   8.22947047   3.55238806
 6.33504932   5.48631365   3.55238806
 7.91881165   2.74315682   3.55238806
 9.50257398   0.00000000   3.55238806
11.08633632  -2.74315682   3.55238806
 6.33504932  10.97262730   3.55238806
 7.91881165   8.22947047   3.55238806
 9.50257398   5.48631365   3.55238806
11.08633632   2.74315682   3.55238806
12.67009865   0.00000000   3.55238806
 0.00000000   0.00000000   7.10477612
 1.58376233  -2.74315682   7.10477612
 3.16752466  -5.48631365   7.10477612
 4.75128699  -8.22947047   7.10477612
 6.33504932 -10.97262730   7.10477612
 1.58376233   2.74315682   7.10477612
 3.16752466   0.00000000   7.10477612
 4.75128699  -2.74315682   7.10477612
 6.33504932  -5.48631365   7.10477612
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
```

```
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
```

```
 6.33504932  -1.82877122  1.77619403
 6.33504932  -3.65754243  1.77619403
 7.91881165  -4.57192804  1.77619403
 7.91881165  -6.40069926  1.77619403
 9.50257398  -7.31508486  1.77619403
 9.50257398  -9.14385608  1.77619403
 4.75128699   6.40069926  1.77619403
 4.75128699   4.57192804  1.77619403
 6.33504932   3.65754243  1.77619403
 6.33504932   1.82877122  1.77619403
 7.91881165   0.91438561  1.77619403
 7.91881165  -0.91438561  1.77619403
 9.50257398  -1.82877122  1.77619403
 9.50257398  -3.65754243  1.77619403
11.08633632  -4.57192804  1.77619403
11.08633632  -6.40069926  1.77619403
 6.33504932   9.14385608  1.77619403
 6.33504932   7.31508486  1.77619403
 7.91881165   6.40069926  1.77619403
 7.91881165   4.57192804  1.77619403
 9.50257398   3.65754243  1.77619403
 9.50257398   1.82877122  1.77619403
11.08633632   0.91438561  1.77619403
11.08633632  -0.91438561  1.77619403
12.67009865  -1.82877122  1.77619403
12.67009865  -3.65754243  1.77619403
 7.91881165  11.88701290  1.77619403
 7.91881165  10.05824169  1.77619403
 9.50257398   9.14385608  1.77619403
 9.50257398   7.31508486  1.77619403
11.08633632   6.40069926  1.77619403
11.08633632   4.57192804  1.77619403
12.67009865   3.65754243  1.77619403
12.67009865   1.82877122  1.77619403
14.25386098   0.91438561  1.77619403
14.25386098  -0.91438561  1.77619403
 1.58376233   0.91438561  5.32858209
 1.58376233  -0.91438561  5.32858209
 3.16752466  -1.82877122  5.32858209
 3.16752466  -3.65754243  5.32858209
 4.75128699  -4.57192804  5.32858209
 4.75128699  -6.40069926  5.32858209
 6.33504932  -7.31508486  5.32858209
 6.33504932  -9.14385608  5.32858209
 7.91881165 -10.05824169  5.32858209
 7.91881165 -11.88701290  5.32858209
 3.16752466   3.65754243  5.32858209
 3.16752466   1.82877122  5.32858209
 4.75128699   0.91438561  5.32858209
 4.75128699  -0.91438561  5.32858209
 6.33504932  -1.82877122  5.32858209
 6.33504932  -3.65754243  5.32858209
 7.91881165  -4.57192804  5.32858209
 7.91881165  -6.40069926  5.32858209
 9.50257398  -7.31508486  5.32858209
 9.50257398  -9.14385608  5.32858209
 4.75128699   6.40069926  5.32858209
 4.75128699   4.57192804  5.32858209
 6.33504932   3.65754243  5.32858209
 6.33504932   1.82877122  5.32858209
 7.91881165   0.91438561  5.32858209
 7.91881165  -0.91438561  5.32858209
```

```
 9.50257398       -1.82877122        5.32858209
 9.50257398       -3.65754243        5.32858209
11.08633632       -4.57192804        5.32858209
11.08633632       -6.40069926        5.32858209
 6.33504932        9.14385608        5.32858209
 6.33504932        7.31508486        5.32858209
 7.91881165        6.40069926        5.32858209
 7.91881165        4.57192804        5.32858209
 9.50257398        3.65754243        5.32858209
 9.50257398        1.82877122        5.32858209
11.08633632        0.91438561        5.32858209
11.08633632       -0.91438561        5.32858209
12.67009865       -1.82877122        5.32858209
12.67009865       -3.65754243        5.32858209
 7.91881165       11.88701290        5.32858209
 7.91881165       10.05824169        5.32858209
 9.50257398        9.14385608        5.32858209
 9.50257398        7.31508486        5.32858209
11.08633632        6.40069926        5.32858209
11.08633632        4.57192804        5.32858209
12.67009865        3.65754243        5.32858209
12.67009865        1.82877122        5.32858209
14.25386098        0.91438561        5.32858209
14.25386098       -0.91438561        5.32858209
 1.58376233        0.91438561        8.88097015
 1.58376233       -0.91438561        8.88097015
 3.16752466       -1.82877122        8.88097015
 3.16752466       -3.65754243        8.88097015
 4.75128699       -4.57192804        8.88097015
 4.75128699       -6.40069926        8.88097015
 6.33504932       -7.31508486        8.88097015
 6.33504932       -9.14385608        8.88097015
 7.91881165      -10.05824169        8.88097015
 7.91881165      -11.88701290        8.88097015
 3.16752466        3.65754243        8.88097015
 3.16752466        1.82877122        8.88097015
 4.75128699        0.91438561        8.88097015
 4.75128699       -0.91438561        8.88097015
 6.33504932       -1.82877122        8.88097015
 6.33504932       -3.65754243        8.88097015
 7.91881165       -4.57192804        8.88097015
 7.91881165       -6.40069926        8.88097015
 9.50257398       -7.31508486        8.88097015
 9.50257398       -9.14385608        8.88097015
 4.75128699        6.40069926        8.88097015
 4.75128699        4.57192804        8.88097015
 6.33504932        3.65754243        8.88097015
 6.33504932        1.82877122        8.88097015
 7.91881165        0.91438561        8.88097015
 7.91881165       -0.91438561        8.88097015
 9.50257398       -1.82877122        8.88097015
 9.50257398       -3.65754243        8.88097015
11.08633632       -4.57192804        8.88097015
11.08633632       -6.40069926        8.88097015
 6.33504932        9.14385608        8.88097015
 6.33504932        7.31508486        8.88097015
 7.91881165        6.40069926        8.88097015
 7.91881165        4.57192804        8.88097015
 9.50257398        3.65754243        8.88097015
 9.50257398        1.82877122        8.88097015
11.08633632        0.91438561        8.88097015
11.08633632       -0.91438561        8.88097015
```

```
 12.67009865  -1.82877122   8.88097015
 12.67009865  -3.65754243   8.88097015
  7.91881165  11.88701290   8.88097015
  7.91881165  10.05824169   8.88097015
  9.50257398   9.14385608   8.88097015
  9.50257398   7.31508486   8.88097015
 11.08633632   6.40069926   8.88097015
 11.08633632   4.57192804   8.88097015
 12.67009865   3.65754243   8.88097015
 12.67009865   1.82877122   8.88097015
 14.25386098   0.91438561   8.88097015
 14.25386098  -0.91438561   8.88097015
  1.58376233   0.91438561  12.43335821
  1.58376233  -0.91438561  12.43335821
  3.16752466  -1.82877122  12.43335821
  3.16752466  -3.65754243  12.43335821
  4.75128699  -4.57192804  12.43335821
  4.75128699  -6.40069926  12.43335821
  6.33504932  -7.31508486  12.43335821
  6.33504932  -9.14385608  12.43335821
  7.91881165 -10.05824169  12.43335821
  7.91881165 -11.88701290  12.43335821
  3.16752466   3.65754243  12.43335821
  3.16752466   1.82877122  12.43335821
  4.75128699   0.91438561  12.43335821
  4.75128699  -0.91438561  12.43335821
  6.33504932  -1.82877122  12.43335821
  6.33504932  -3.65754243  12.43335821
  7.91881165  -4.57192804  12.43335821
  7.91881165  -6.40069926  12.43335821
  9.50257398  -7.31508486  12.43335821
  9.50257398  -9.14385608  12.43335821
  4.75128699   6.40069926  12.43335821
  4.75128699   4.57192804  12.43335821
  6.33504932   3.65754243  12.43335821
  6.33504932   1.82877122  12.43335821
  7.91881165   0.91438561  12.43335821
  7.91881165  -0.91438561  12.43335821
  9.50257398  -1.82877122  12.43335821
  9.50257398  -3.65754243  12.43335821
 11.08633632  -4.57192804  12.43335821
 11.08633632  -6.40069926  12.43335821
  6.33504932   9.14385608  12.43335821
  6.33504932   7.31508486  12.43335821
  7.91881165   6.40069926  12.43335821
  7.91881165   4.57192804  12.43335821
  9.50257398   3.65754243  12.43335821
  9.50257398   1.82877122  12.43335821
 11.08633632   0.91438561  12.43335821
 11.08633632  -0.91438561  12.43335821
 12.67009865  -1.82877122  12.43335821
 12.67009865  -3.65754243  12.43335821
  7.91881165  11.88701290  12.43335821
  7.91881165  10.05824169  12.43335821
  9.50257398   9.14385608  12.43335821
  9.50257398   7.31508486  12.43335821
 11.08633632   6.40069926  12.43335821
 11.08633632   4.57192804  12.43335821
 12.67009865   3.65754243  12.43335821
 12.67009865   1.82877122  12.43335821
 14.25386098   0.91438561  12.43335821
 14.25386098  -0.91438561  12.43335821
```

```
      1.58376233         0.91438561        15.98574627
      1.58376233        -0.91438561        15.98574627
      3.16752466        -1.82877122        15.98574627
      3.16752466        -3.65754243        15.98574627
      4.75128699        -4.57192804        15.98574627
      4.75128699        -6.40069926        15.98574627
      6.33504932        -7.31508486        15.98574627
      6.33504932        -9.14385608        15.98574627
      7.91881165       -10.05824169        15.98574627
      7.91881165       -11.88701290        15.98574627
      3.16752466         3.65754243        15.98574627
      3.16752466         1.82877122        15.98574627
      4.75128699         0.91438561        15.98574627
      4.75128699        -0.91438561        15.98574627
      6.33504932        -1.82877122        15.98574627
      6.33504932        -3.65754243        15.98574627
      7.91881165        -4.57192804        15.98574627
      7.91881165        -6.40069926        15.98574627
      9.50257398        -7.31508486        15.98574627
      9.50257398        -9.14385608        15.98574627
      4.75128699         6.40069926        15.98574627
      4.75128699         4.57192804        15.98574627
      6.33504932         3.65754243        15.98574627
      6.33504932         1.82877122        15.98574627
      7.91881165         0.91438561        15.98574627
      7.91881165        -0.91438561        15.98574627
      9.50257398        -1.82877122        15.98574627
      9.50257398        -3.65754243        15.98574627
     11.08633632        -4.57192804        15.98574627
     11.08633632        -6.40069926        15.98574627
      6.33504932         9.14385608        15.98574627
      6.33504932         7.31508486        15.98574627
      7.91881165         6.40069926        15.98574627
      7.91881165         4.57192804        15.98574627
      9.50257398         3.65754243        15.98574627
      9.50257398         1.82877122        15.98574627
     11.08633632         0.91438561        15.98574627
     11.08633632        -0.91438561        15.98574627
     12.67009865        -1.82877122        15.98574627
     12.67009865        -3.65754243        15.98574627
      7.91881165        11.88701290        15.98574627
      7.91881165        10.05824169        15.98574627
      9.50257398         9.14385608        15.98574627
      9.50257398         7.31508486        15.98574627
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
   7.91881   0.91439  17.76194
```

Listing 29: Structural input file for configuration: 5x5x5 O Zr ring.

5x5x5_Zr_inter POSCAR

```
# Zr1 B2
1.000000
      7.91881165       -13.71578412         0.00000000
      7.91881165        13.71578412         0.00000000
      0.00000000         0.00000000        17.76194030
```

```
 Zr  B
   126     249
Cartesian
      0.00000000        0.00000000        0.00000000
      1.58376233       -2.74315682        0.00000000
      3.16752466       -5.48631365        0.00000000
      4.75128699       -8.22947047        0.00000000
      6.33504932      -10.97262730        0.00000000
      1.58376233        2.74315682        0.00000000
      3.16752466        0.00000000        0.00000000
      4.75128699       -2.74315682        0.00000000
      6.33504932       -5.48631365        0.00000000
      7.91881165       -8.22947047        0.00000000
      3.16752466        5.48631365        0.00000000
      4.75128699        2.74315682        0.00000000
      6.33504932        0.00000000        0.00000000
      7.91881165       -2.74315682        0.00000000
      9.50257398       -5.48631365        0.00000000
      4.75128699        8.22947047        0.00000000
      6.33504932        5.48631365        0.00000000
      7.91881165        2.74315682        0.00000000
      9.50257398        0.00000000        0.00000000
     11.08633632       -2.74315682        0.00000000
      6.33504932       10.97262730        0.00000000
      7.91881165        8.22947047        0.00000000
      9.50257398        5.48631365        0.00000000
     11.08633632        2.74315682        0.00000000
     12.67009865        0.00000000        0.00000000
      0.00000000        0.00000000        3.55238806
      1.58376233       -2.74315682        3.55238806
      3.16752466       -5.48631365        3.55238806
      4.75128699       -8.22947047        3.55238806
      6.33504932      -10.97262730        3.55238806
      1.58376233        2.74315682        3.55238806
      3.16752466        0.00000000        3.55238806
      4.75128699       -2.74315682        3.55238806
      6.33504932       -5.48631365        3.55238806
      7.91881165       -8.22947047        3.55238806
      3.16752466        5.48631365        3.55238806
      4.75128699        2.74315682        3.55238806
      6.33504932        0.00000000        3.55238806
      7.91881165       -2.74315682        3.55238806
      9.50257398       -5.48631365        3.55238806
      4.75128699        8.22947047        3.55238806
      6.33504932        5.48631365        3.55238806
      7.91881165        2.74315682        3.55238806
      9.50257398        0.00000000        3.55238806
     11.08633632       -2.74315682        3.55238806
      6.33504932       10.97262730        3.55238806
      7.91881165        8.22947047        3.55238806
      9.50257398        5.48631365        3.55238806
     11.08633632        2.74315682        3.55238806
     12.67009865        0.00000000        3.55238806
      0.00000000        0.00000000        7.10477612
      1.58376233       -2.74315682        7.10477612
      3.16752466       -5.48631365        7.10477612
      4.75128699       -8.22947047        7.10477612
      6.33504932      -10.97262730        7.10477612
      1.58376233        2.74315682        7.10477612
      3.16752466        0.00000000        7.10477612
      4.75128699       -2.74315682        7.10477612
      6.33504932       -5.48631365        7.10477612
```

```
 7.91881165  -8.22947047   7.10477612
 3.16752466   5.48631365   7.10477612
 4.75128699   2.74315682   7.10477612
 6.33504932   0.00000000   7.10477612
 7.91881165  -2.74315682   7.10477612
 9.50257398  -5.48631365   7.10477612
 4.75128699   8.22947047   7.10477612
 6.33504932   5.48631365   7.10477612
 7.91881165   2.74315682   7.10477612
 9.50257398   0.00000000   7.10477612
11.08633632  -2.74315682   7.10477612
 6.33504932  10.97262730   7.10477612
 7.91881165   8.22947047   7.10477612
 9.50257398   5.48631365   7.10477612
11.08633632   2.74315682   7.10477612
12.67009865   0.00000000   7.10477612
 0.00000000   0.00000000  10.65716418
 1.58376233  -2.74315682  10.65716418
 3.16752466  -5.48631365  10.65716418
 4.75128699  -8.22947047  10.65716418
 6.33504932 -10.97262730  10.65716418
 1.58376233   2.74315682  10.65716418
 3.16752466   0.00000000  10.65716418
 4.75128699  -2.74315682  10.65716418
 6.33504932  -5.48631365  10.65716418
 7.91881165  -8.22947047  10.65716418
 3.16752466   5.48631365  10.65716418
 4.75128699   2.74315682  10.65716418
 6.33504932   0.00000000  10.65716418
 7.91881165  -2.74315682  10.65716418
 9.50257398  -5.48631365  10.65716418
 4.75128699   8.22947047  10.65716418
 6.33504932   5.48631365  10.65716418
 7.91881165   2.74315682  10.65716418
 9.50257398   0.00000000  10.65716418
11.08633632  -2.74315682  10.65716418
 6.33504932  10.97262730  10.65716418
 7.91881165   8.22947047  10.65716418
 9.50257398   5.48631365  10.65716418
11.08633632   2.74315682  10.65716418
12.67009865   0.00000000  10.65716418
 0.00000000   0.00000000  14.20955224
 1.58376233  -2.74315682  14.20955224
 3.16752466  -5.48631365  14.20955224
 4.75128699  -8.22947047  14.20955224
 6.33504932 -10.97262730  14.20955224
 1.58376233   2.74315682  14.20955224
 3.16752466   0.00000000  14.20955224
 4.75128699  -2.74315682  14.20955224
 6.33504932  -5.48631365  14.20955224
 7.91881165  -8.22947047  14.20955224
 3.16752466   5.48631365  14.20955224
 4.75128699   2.74315682  14.20955224
 6.33504932   0.00000000  14.20955224
 7.91881165  -2.74315682  14.20955224
 9.50257398  -5.48631365  14.20955224
 4.75128699   8.22947047  14.20955224
 6.33504932   5.48631365  14.20955224
 7.91881165   2.74315682  14.20955224
 9.50257398   0.00000000  14.20955224
11.08633632  -2.74315682  14.20955224
 6.33504932  10.97262730  14.20955224
```

```
 7.91881165   8.22947047  14.20955224
 9.50257398   5.48631365  14.20955224
11.08633632   2.74315682  14.20955224
12.67009865   0.00000000  14.20955224
 1.58376233   0.91438561   1.77619403
 1.58376233  -0.91438561   1.77619403
 3.16752466  -1.82877122   1.77619403
 3.16752466  -3.65754243   1.77619403
 4.75128699  -4.57192804   1.77619403
 4.75128699  -6.40069926   1.77619403
 6.33504932  -7.31508486   1.77619403
 6.33504932  -9.14385608   1.77619403
 7.91881165 -10.05824169   1.77619403
 7.91881165 -11.88701290   1.77619403
 3.16752466   3.65754243   1.77619403
 3.16752466   1.82877122   1.77619403
 4.75128699   0.91438561   1.77619403
 4.75128699  -0.91438561   1.77619403
 6.33504932  -1.82877122   1.77619403
 6.33504932  -3.65754243   1.77619403
 7.91881165  -4.57192804   1.77619403
 7.91881165  -6.40069926   1.77619403
 9.50257398  -7.31508486   1.77619403
 9.50257398  -9.14385608   1.77619403
 4.75128699   6.40069926   1.77619403
 4.75128699   4.57192804   1.77619403
 6.33504932   3.65754243   1.77619403
 6.33504932   1.82877122   1.77619403
 7.91881165   0.91438561   1.77619403
 7.91881165  -0.91438561   1.77619403
 9.50257398  -1.82877122   1.77619403
 9.50257398  -3.65754243   1.77619403
11.08633632  -4.57192804   1.77619403
11.08633632  -6.40069926   1.77619403
 6.33504932   9.14385608   1.77619403
 6.33504932   7.31508486   1.77619403
 7.91881165   6.40069926   1.77619403
 7.91881165   4.57192804   1.77619403
 9.50257398   3.65754243   1.77619403
 9.50257398   1.82877122   1.77619403
11.08633632   0.91438561   1.77619403
11.08633632  -0.91438561   1.77619403
12.67009865  -1.82877122   1.77619403
12.67009865  -3.65754243   1.77619403
 7.91881165  11.88701290   1.77619403
 7.91881165  10.05824169   1.77619403
 9.50257398   9.14385608   1.77619403
 9.50257398   7.31508486   1.77619403
11.08633632   6.40069926   1.77619403
11.08633632   4.57192804   1.77619403
12.67009865   3.65754243   1.77619403
12.67009865   1.82877122   1.77619403
14.25386098   0.91438561   1.77619403
14.25386098  -0.91438561   1.77619403
 1.58376233   0.91438561   5.32858209
 1.58376233  -0.91438561   5.32858209
 3.16752466  -1.82877122   5.32858209
 3.16752466  -3.65754243   5.32858209
 4.75128699  -4.57192804   5.32858209
 4.75128699  -6.40069926   5.32858209
 6.33504932  -7.31508486   5.32858209
 6.33504932  -9.14385608   5.32858209
```

```
 7.91881165  -10.05824169   5.32858209
 7.91881165  -11.88701290   5.32858209
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 3.16752466    1.82877122   5.32858209
 4.75128699    0.91438561   5.32858209
 4.75128699   -0.91438561   5.32858209
 6.33504932   -1.82877122   5.32858209
 6.33504932   -3.65754243   5.32858209
 7.91881165   -4.57192804   5.32858209
 7.91881165   -6.40069926   5.32858209
 9.50257398   -7.31508486   5.32858209
 9.50257398   -9.14385608   5.32858209
 4.75128699    6.40069926   5.32858209
 4.75128699    4.57192804   5.32858209
 6.33504932    3.65754243   5.32858209
 6.33504932    1.82877122   5.32858209
 7.91881165    0.91438561   5.32858209
 7.91881165   -0.91438561   5.32858209
 9.50257398   -1.82877122   5.32858209
 9.50257398   -3.65754243   5.32858209
11.08633632   -4.57192804   5.32858209
11.08633632   -6.40069926   5.32858209
 6.33504932    9.14385608   5.32858209
 6.33504932    7.31508486   5.32858209
 7.91881165    6.40069926   5.32858209
 7.91881165    4.57192804   5.32858209
 9.50257398    3.65754243   5.32858209
 9.50257398    1.82877122   5.32858209
11.08633632    0.91438561   5.32858209
11.08633632   -0.91438561   5.32858209
12.67009865   -1.82877122   5.32858209
12.67009865   -3.65754243   5.32858209
 7.91881165   11.88701290   5.32858209
 7.91881165   10.05824169   5.32858209
 9.50257398    9.14385608   5.32858209
 9.50257398    7.31508486   5.32858209
11.08633632    6.40069926   5.32858209
11.08633632    4.57192804   5.32858209
12.67009865    3.65754243   5.32858209
12.67009865    1.82877122   5.32858209
14.25386098    0.91438561   5.32858209
14.25386098   -0.91438561   5.32858209
 1.58376233    0.91438561   8.88097015
 1.58376233   -0.91438561   8.88097015
 3.16752466   -1.82877122   8.88097015
 3.16752466   -3.65754243   8.88097015
 4.75128699   -4.57192804   8.88097015
 4.75128699   -6.40069926   8.88097015
 6.33504932   -7.31508486   8.88097015
 6.33504932   -9.14385608   8.88097015
 7.91881165  -10.05824169   8.88097015
 7.91881165  -11.88701290   8.88097015
 3.16752466    3.65754243   8.88097015
 3.16752466    1.82877122   8.88097015
 4.75128699    0.91438561   8.88097015
 4.75128699   -0.91438561   8.88097015
 6.33504932   -1.82877122   8.88097015
 6.33504932   -3.65754243   8.88097015
 7.91881165   -4.57192804   8.88097015
 7.91881165   -6.40069926   8.88097015
 9.50257398   -7.31508486   8.88097015
 9.50257398   -9.14385608   8.88097015
```

```
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 4.75128699   4.57192804   8.88097015
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 6.33504932   1.82877122   8.88097015
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 7.91881165  -0.91438561   8.88097015
 9.50257398  -1.82877122   8.88097015
 9.50257398  -3.65754243   8.88097015
11.08633632  -4.57192804   8.88097015
11.08633632  -6.40069926   8.88097015
 6.33504932   9.14385608   8.88097015
 6.33504932   7.31508486   8.88097015
 7.91881165   6.40069926   8.88097015
 7.91881165   4.57192804   8.88097015
 9.50257398   3.65754243   8.88097015
 9.50257398   1.82877122   8.88097015
11.08633632   0.91438561   8.88097015
11.08633632  -0.91438561   8.88097015
12.67009865  -1.82877122   8.88097015
12.67009865  -3.65754243   8.88097015
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 9.50257398   9.14385608   8.88097015
 9.50257398   7.31508486   8.88097015
11.08633632   6.40069926   8.88097015
11.08633632   4.57192804   8.88097015
12.67009865   3.65754243   8.88097015
12.67009865   1.82877122   8.88097015
14.25386098   0.91438561   8.88097015
14.25386098  -0.91438561   8.88097015
 1.58376233   0.91438561  12.43335821
 1.58376233  -0.91438561  12.43335821
 3.16752466  -1.82877122  12.43335821
 3.16752466  -3.65754243  12.43335821
 4.75128699  -4.57192804  12.43335821
 4.75128699  -6.40069926  12.43335821
 6.33504932  -7.31508486  12.43335821
 6.33504932  -9.14385608  12.43335821
 7.91881165 -10.05824169  12.43335821
 7.91881165 -11.88701290  12.43335821
 3.16752466   3.65754243  12.43335821
 3.16752466   1.82877122  12.43335821
 4.75128699   0.91438561  12.43335821
 4.75128699  -0.91438561  12.43335821
 6.33504932  -1.82877122  12.43335821
 6.33504932  -3.65754243  12.43335821
 7.91881165  -4.57192804  12.43335821
 7.91881165  -6.40069926  12.43335821
 9.50257398  -7.31508486  12.43335821
 9.50257398  -9.14385608  12.43335821
 4.75128699   6.40069926  12.43335821
 4.75128699   4.57192804  12.43335821
 6.33504932   3.65754243  12.43335821
 6.33504932   1.82877122  12.43335821
 7.91881165   0.91438561  12.43335821
 7.91881165  -0.91438561  12.43335821
 9.50257398  -1.82877122  12.43335821
 9.50257398  -3.65754243  12.43335821
11.08633632  -4.57192804  12.43335821
11.08633632  -6.40069926  12.43335821
 6.33504932   9.14385608  12.43335821
 6.33504932   7.31508486  12.43335821
```

```
 7.91881165  6.40069926 12.43335821
 7.91881165  4.57192804 12.43335821
 9.50257398  3.65754243 12.43335821
 9.50257398  1.82877122 12.43335821
11.08633632  0.91438561 12.43335821
11.08633632 -0.91438561 12.43335821
12.67009865 -1.82877122 12.43335821
12.67009865 -3.65754243 12.43335821
 7.91881165 11.88701290 12.43335821
 7.91881165 10.05824169 12.43335821
 9.50257398  9.14385608 12.43335821
 9.50257398  7.31508486 12.43335821
11.08633632  6.40069926 12.43335821
11.08633632  4.57192804 12.43335821
12.67009865  3.65754243 12.43335821
12.67009865  1.82877122 12.43335821
14.25386098  0.91438561 12.43335821
14.25386098 -0.91438561 12.43335821
 1.58376233  0.91438561 15.98574627
 1.58376233 -0.91438561 15.98574627
 3.16752466 -1.82877122 15.98574627
 3.16752466 -3.65754243 15.98574627
 4.75128699 -4.57192804 15.98574627
 4.75128699 -6.40069926 15.98574627
 6.33504932 -7.31508486 15.98574627
 6.33504932 -9.14385608 15.98574627
 7.91881165 -10.05824169 15.98574627
 7.91881165 -11.88701290 15.98574627
 3.16752466  3.65754243 15.98574627
 3.16752466  1.82877122 15.98574627
 4.75128699  0.91438561 15.98574627
 4.75128699 -0.91438561 15.98574627
 6.33504932 -1.82877122 15.98574627
 6.33504932 -3.65754243 15.98574627
 7.91881165 -4.57192804 15.98574627
 7.91881165 -6.40069926 15.98574627
 9.50257398 -7.31508486 15.98574627
 9.50257398 -9.14385608 15.98574627
 4.75128699  6.40069926 15.98574627
 4.75128699  4.57192804 15.98574627
 6.33504932  3.65754243 15.98574627
 6.33504932  1.82877122 15.98574627
 7.91881165  0.91438561 15.98574627
 7.91881165 -0.91438561 15.98574627
 9.50257398 -1.82877122 15.98574627
 9.50257398 -3.65754243 15.98574627
11.08633632 -4.57192804 15.98574627
11.08633632 -6.40069926 15.98574627
 6.33504932  9.14385608 15.98574627
 6.33504932  7.31508486 15.98574627
 7.91881165  6.40069926 15.98574627
 7.91881165  4.57192804 15.98574627
 9.50257398  3.65754243 15.98574627
 9.50257398  1.82877122 15.98574627
11.08633632  0.91438561 15.98574627
11.08633632 -0.91438561 15.98574627
12.67009865 -1.82877122 15.98574627
12.67009865 -3.65754243 15.98574627
 7.91881165 11.88701290 15.98574627
 7.91881165 10.05824169 15.98574627
 9.50257398  9.14385608 15.98574627
 9.50257398  7.31508486 15.98574627
```

```
     11.08633632         6.40069926        15.98574627
     11.08633632         4.57192804        15.98574627
     12.67009865         3.65754243        15.98574627
     12.67009865         1.82877122        15.98574627
     14.25386098         0.91438561        15.98574627
     14.25386098        -0.91438561        15.98574627
```

Listing 30: Structural input file for configuration: 5x5x5 Zr inter.