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# Semiconducting phase of hafnium dioxide under high pressure: a theoretical study by quasi-particle GW calculations

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**Keywords:** hafnium dioxide, semiconductor, high pressure, density functional theory

## Abstract

The phase stability of the hafnium dioxide compounds  $\text{HfO}_2$ , a novel material with a wide range of application due to its versatility and biocompatibility, is predicted to be achievable by using evolutionary technique, based on first-principles calculations. Herein, the candidate structure of  $\text{HfO}_2$  is revealed to adopt a tetragonal structure under high-pressure phase with  $P4/nmm$  space group. This evidently confirms the stability of the  $\text{HfO}_2$  structures, since the decomposition into the component elements under pressure does not occur until the pressure is at least 200 GPa. Moreover, phonon calculations can confirm that the  $P4/nmm$  structure is dynamically stable. The  $P4/nmm$  structure is mainly attributed to the semiconducting property within using the Perdew–Burke–Ernzerhof, the modified Becke–Johnson exchange potential in combination with the generalized gradient approximations, and the quasi-particle GW approximation, respectively. Our calculation manifests that the  $P4/nmm$  structure is likely to be metal above 200 GPa, arising particularly from GW approximation. The remarkable results of this work provide more understanding of the high-pressure structure for designing metal-oxide-based semiconducting materials.

## 1. Introduction

Hafnium oxide  $\text{HfO}_2$  is a remarkable material with various applications. Currently, the Hafnium oxide-based material is mainly used as the ideal memory material, [1–5] i.e. ferroelectric Si-doped  $\text{HfO}_2$  [6–9] due to its ferroelectric property. Moreover, as a part of solid oxide-deficient technology,  $\text{HfO}_2$  is also an attractive material for resistive-switching memories [10–14]. Under a broad range of pressure,  $\text{HfO}_2$  becomes a superhard material [15–17]. Its physical properties such as structural, electrical, optical, and elastic properties have recently been investigated by computational study [17]. Also,  $\text{HfO}_2$  is considered an indirect band gap semiconductor with the band gap of 4.62 eV. Therefore, it is expected that  $\text{HfO}_2$  could possibly be utilized as metal-oxide-semiconductor devices in the upcoming generations.

Moreover,  $\text{HfO}_2$  has been fundamentally studied under high pressure. The phase transition has been demonstrated experimentally by the Raman spectra and x-ray-diffraction technique [18]. As a result, it displayed a monoclinic structure with the space group  $P2_1/c$ , then transformed into an orthorhombic I with the space group  $Pbca$  at 10.2 GPa, and finally at 37 GPa, it transformed into an orthorhombic II with the space group  $Pnma$ . The structural behavior of the  $Pnma$  structure of  $\text{HfO}_2$  was investigated at each pressure [19]. It was discovered that the  $Pnma$  structure exhibits dynamical stability, but the structure is thermodynamically

unstable. The meta stability can be observed up to at least 120 GPa. Additionally, it should be noted that the *Pnma* structure exhibits semiconductivity with the band gap of 3.36, eV. Interestingly, there is no previous report on the crystal structure of HfO<sub>2</sub> above 120 GPa. Therefore, the existence of a stable structure with novel property of HfO<sub>2</sub> above 120 GPa could be anticipated.

In this work, HfO<sub>2</sub> will be explored by the evolutionary techniques, based on density functional theory, to predict the novel structure as a function of pressure. Following this, the main attention is turned to the prediction of candidate structures under up to 200 GPa of pressure. As a result of the structural prediction, the stability of the candidate structures will be examined by considering the formation enthalpy. From the results, the existence of the structure confirms the composition of binary hafnium oxides, which is HfO<sub>2</sub>, with respect to pure Hf and O. In other words, the material does not decompose into pure elements under at least 200 GPa of pressure. The remarkable result of the evolutionary techniques displayed a candidate high-pressure phase: a tetragonal structure with a space group of P4/nmm. By considering the physical properties, the P4/nmm exhibits semiconductivity. These findings provide crucial details for fundamental understanding of the structural behaviour and the electronic properties of the HfO<sub>2</sub> at each pressure. Note also that our work provides only HfO<sub>2</sub>. It is because other Hf-O compounds clearly explore further investigation by Zhang *et al* [19].

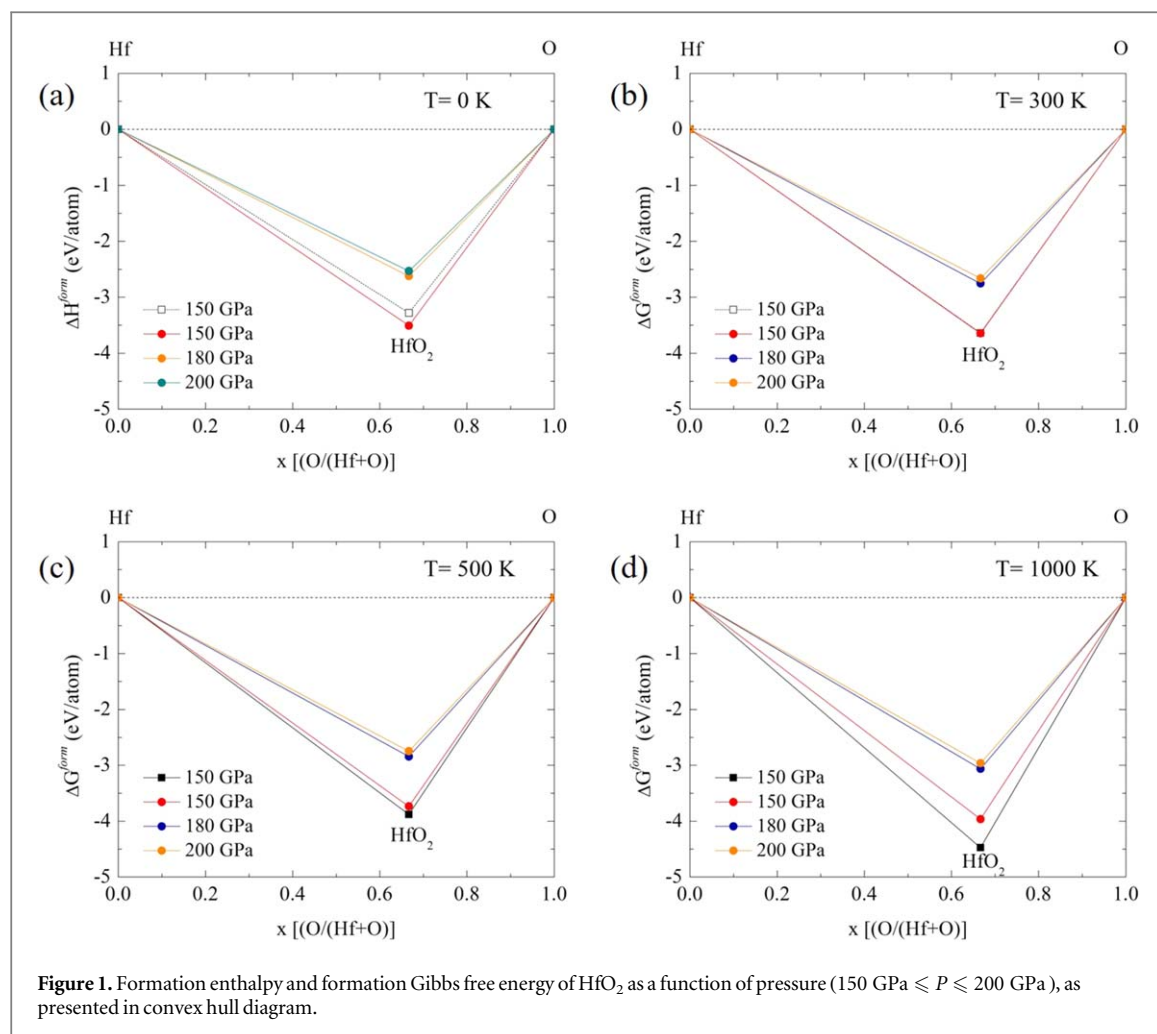
## 2. Methods

The computation implemented the universal Structure Predictor: Evolutionary Xtallography (USPEX) [20] and the Vienna *ab initio* simulation package (VASP) [21] which utilizes the density functional theory. In all subsequent generations, the random symmetric algorithm employed 40% heredity, 20% random symmetric, 20% soft mutation, and 20% transmutation operators. We then studied the system under the pressure range of 150 to 200 GPa with up to four formula units. There are 1702 configurations which possess the lowest enthalpy in 56 consecutive generations. A convergence test on plane-wave basis set was performed. As a result, the cutoff energy of 700 eV was achieved. This value is used for the formation enthalpy carried on the generalized gradient approximation of the Perdew–Burke–Ernzerhof (GGA-PBE) functional [22]. The projector augmented wave (PAW) method [23] and the conjugate gradient scheme, both implemented in the VASP code, [21] were used for the calculation of the ground state energy. The pseudocore radii of Hf and O are 2.4 Bohr and 1.1 Bohr, respectively, which are small enough to ensure that no overlap of spheres will occur under compressed conditions. The tetragonal structure was calculated with an initial Brillouin-zone (BZ) sampling grid of spacing  $2\pi \times 0.02 \text{ \AA}^{-1}$  in order to guarantee the convergence of the derived ground-state energy. To confirm the dynamical stability, the structure was calculated by using the *ab initio* lattice dynamics with the supercell approach, as implemented in the VASP code together with the PHONOPY package [24]. As for the density of states, the modified Becke–Johnson (mBJ) exchange potential [25] with the GGA functional was used to fully take into account the energy gap. To further investigate the energy gap, the tetragonal structure was performed a self-energy  $\Sigma$  of a many-body system of electrons, also known as GW approximation [26–29]. One of the well-known GW approximation, the technical details of how the GW approximation is implemented have been described extensively in [28, 29]. The present work has been calculated within a single-shot calculation ( $G_0W_0$ ) by neglecting all off-diagonal matrix elements of the self-energy  $\Sigma$  as well as performing a Taylor expansion of the self-energy  $\Sigma$  around the quasiparticle eigenvalues.

## 3. Results and discussion

The formation enthalpy of HfO<sub>2</sub> is presented in the convex hulls, as shown in figure 1, the possibility of HfO<sub>2</sub> existence under compression can be verified. We first investigated the thermodynamic stability from 150 to 300 GPa by using first-principles calculations. It should be noted that our calculations were performed at a temperature of 0 K, indicating that the enthalpy can confirm a phase stability under high pressure [30–38]. This is due to the fact that there is no entropy contribution. As a result, the relationship between pure elements Hf and O displayed the formation of HfO<sub>2</sub>. We considered the compositions of HfO<sub>2</sub>, bcc-Hf [39] and C2/m-O [40]. The stability of HfO<sub>2</sub> is presented within the connected lower convex wrapper, indicating that there is new high-pressure phase found above 150 GPa: the tetragonal structure with the space group of P4/nmm. Considering the pressure of 150 GPa, the aforementioned theoretical findings manifested that the *Pnma* structure is a meta-stable structure, and it is in good agreement with those previously reported by Zhang *et al* [19]. Moreover, we further explored the P4/nmm and *Pnma* structures by considering entropy *S* contribution, which is obtained as

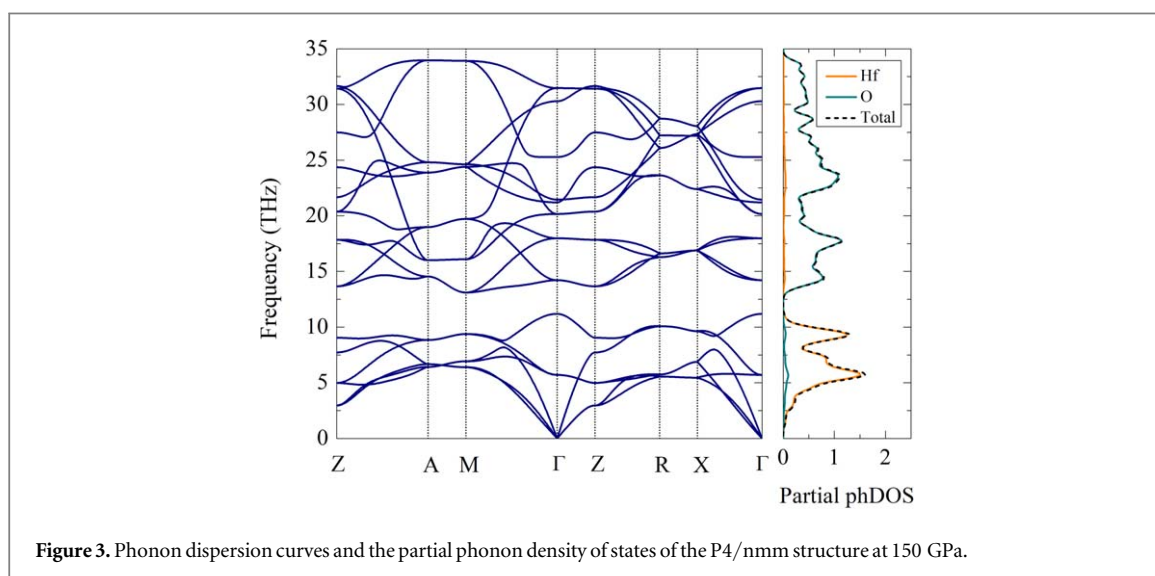
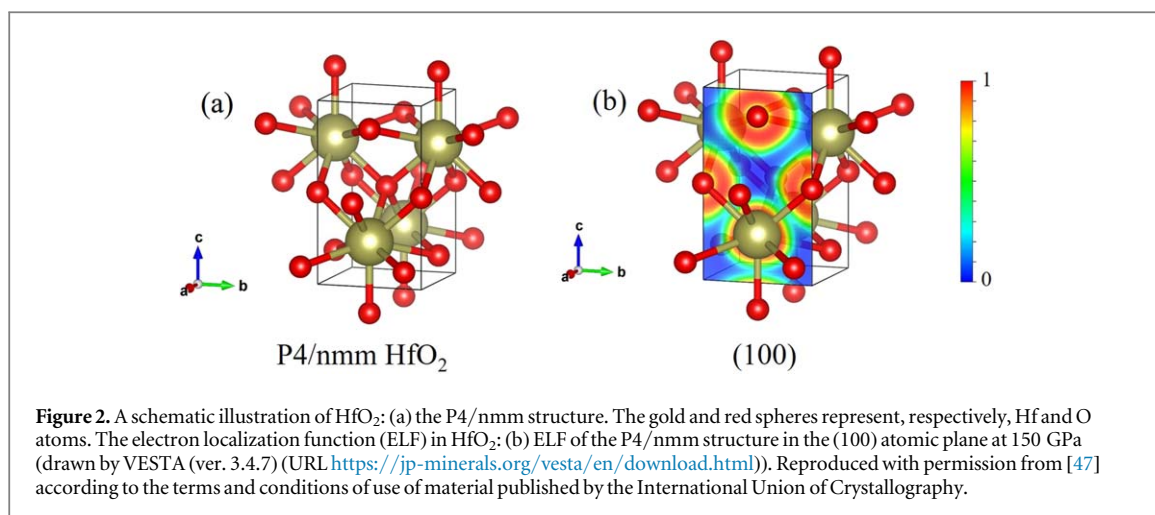
$$S = -k_B \sum_{\nu, q} \ln[1 - \exp(-\hbar\omega_{\nu, q}/k_B T)], \quad (1)$$



where  $\nu$  and  $q$  are band index and the wave vector, respectively.  $\omega$  is the phonon frequency at  $\nu$  and  $q$ .  $T$  is temperature.  $k_B$  and  $\hbar$  are the Boltzmann constant and the reduced Planck constant, respectively. The relative Gibbs free energy showed that the  $P4/nmm$  structure is thermodynamically stable favored over the  $Pnma$  structure by approximately 0.01 eV at a temperature 300 K and a pressure of 150 GPa. As the temperature is increased, it can see that the  $Pnma$  structure is thermodynamically stable at a temperature of 500 K and 1000 K. To understand the structural behavior, it should be noted that the entropy  $S$  increased with increasing temperature. We therefore suggested that the  $Pnma$  structure stable structure depended on the term of  $-TS$ . Here, we suggested that the  $Pnma$  structure is a high-temperature phase. The  $Pnma$  structure, however, beyond the scope of this work, and the issue clearly deserves further investigation—for example, the issue of the dynamical stability at high temperature and electronic properties investigation. Subsequently, the convex hulls showed that the  $Pnma$  structure is holding the meta-stable structure with respect to the  $P4/nmm$  structure. Therefore, it can be implied that the  $P4/nmm$  structure is thermodynamically stable and is favored over the  $Pnma$  by neglecting entropy based on the density functional theory, the formation enthalpy alone is sufficient to confirm phase stability at the temperature of 0 K. Focusing on the  $P4/nmm$  structure, the structure is stable up to at least 200 GPa. Interestingly, the new high-pressure structures do not decompose into pure elements up to at least 200 GPa, resulting in the evidence of phase stability in  $\text{HfO}_2$ .

The possibility of finding an electron in the neighboring space of  $\text{HfO}_2$  can be measured by the electron localization function (ELF) [41], as reported in figure 2, where the structure of  $\text{HfO}_2$  is presented as shown in figure 2 (a). The tendency of ELF in  $\text{HfO}_2$  is described by the uniform distribution of electron gas with the same density [31, 32, 38, 42–46]. For the  $P4/nmm$  structure, the calculated ELF reveals a set of chemical bonding at the pressure of 150 GPa. The distances between the first (Hf-O) and second (O-O) nearest neighbors (NN) read 1.9374 Å, and 2.3477 Å, respectively. As a result of the  $P4/nmm$  structure, it can be observed that the electron would accumulate around the Hf and O atoms, respectively. It should be noted, however, that the O atoms are not likely to bond.

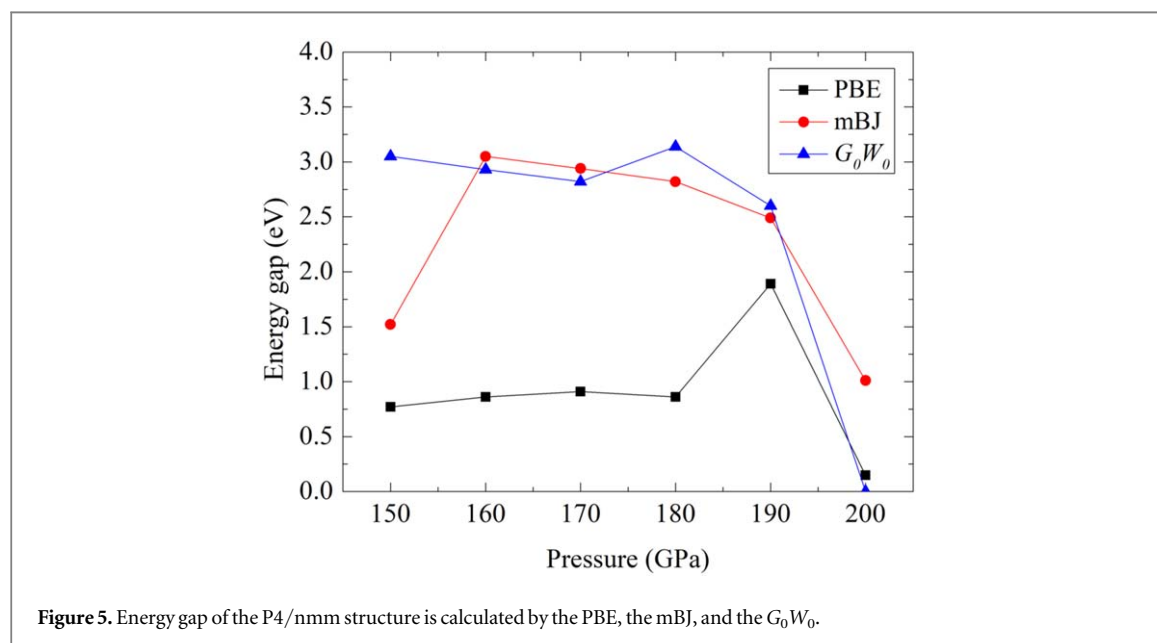
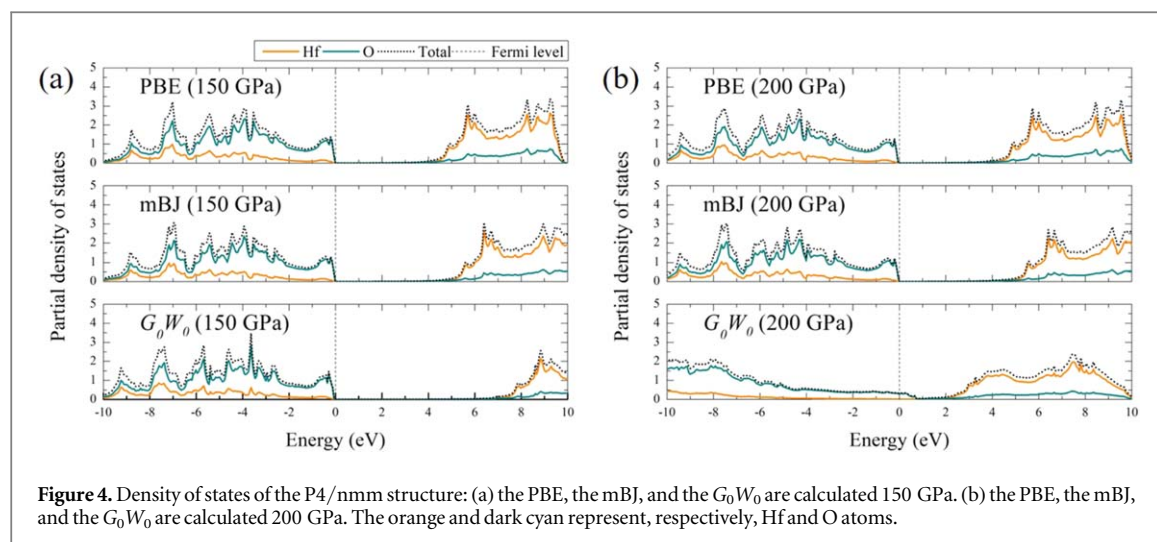
The dynamical stability of the  $P4/nmm$  structure can be confirmed by considering the phonon calculation. We investigated the structures which was obtained from the relative enthalpy calculations and discovered that the two new high-pressure structures exhibited negative enthalpies of formation relative to Hf and O; however, it



is not enough to guarantee the thermodynamic stability. As a result, the  $P4/nmm$  structure is dynamically stable at a pressure of 150 GPa, as shown in figure 3. It is because the structures lack the imaginary frequencies that the  $P4/nmm$  structure is thermodynamically stable.

We will now discuss electronic property of  $\text{HfO}_2$  which is shown in figure 4, as implemented in the density of states (DOS). The DOS has been extensively studied the structural behaviour in several materials. Also, the DOS has been reported in the literature that as the compound systems are useful in achieving in electronic structure. For this reason, it should be noted that, in [48–50] Here, it can be observed that the  $P4/nmm$  structure is semiconductor. Following this, a structural property indicates that, in the PBE method, band gap semiconductors with energy gap of 0.77 eV (figure 4(a)). By taking into consideration the fact that the performance of mBJ for the semiconducting property is more accurate as the calculated energy gaps precision would be similar to the hybrid functional, the mBJ method is likely to solution in energy gap of 1.52 eV. By investigating the energy gap, we have chosen to use GW approximation within a single-shot calculation ( $G_0W_0$ ). At this stage, the  $G_0W_0$  method displayed a large energy gap of 3.05 eV as shown in figure 5. Therefore, it is mentioned that in the PBE method, the energy gap is likely to be underestimated. With increasing pressure, the PBE method shown that the band gap semiconductors with energy gap of 0.15 eV. Also, the estimated the band gap semiconductors is still large in the  $P4/nmm$  structure with energy gap of 1.01 eV by using the mBJ method at a pressure of 200 GPa, as shown in figure 4(b). Interestingly, the remarkable result of the  $G_0W_0$  method displayed that the  $P4/nmm$  structure is metal because there are electrons occupied at the Fermi level (figure 4(b)). Besides, we provide for comparison the values of energy gap evaluated by a different set of parameters, as shown in table 1. It should note that previous calculations and experimental data are revealed the energy gap of the other phases because our work calculated the  $P4/nmm$  structure at high pressure and experimental studies do not yet provide the energy gap above 150 GPa. Therefore, we proposed the theoretical result of the  $P4/nmm$  structure which may guild further experimental studies.





Yet, a more significant change in structural behavior is observed when the pressure increased. As mentioned above, the discovery of apparent metallicity prompts us to further study. It is worth mentioning again that the P4/nmm structure is likely to be metal at a pressure of 200 GPa. Herein, we consider the energy gap as a function of pressure from 150 GPa to 200 GPa. Firstly, the PBE method shown that the estimated energy gap increased gradually from 150 GPa to 180 GPa. Next, the energy gap rose dramatically at a pressure of 190 GPa. After that, the energy gap decreased rapidly at a pressure of 200 GPa. For the case of the mBJ method, the energy gap increased suddenly from 150 GPa to 160 GPa. Then, there was a gradual decrease to 190 GPa, and it decreased suddenly at a pressure of 200 GPa. By employing the  $G_0W_0$  method, our results reveal that, arising particularly from a single-shot calculation, the estimated energy gap decreased gradually from 150 GPa to 170 GPa. Then, we found that it reached a peak of 3.14 eV at a pressure of 180 GPa. After that, the energy gap decreased suddenly from 190 GPa to 200 GPa. These analyses, based on our findings showing the P4/nmm structure accepted to be metallicity above 200 GPa. Consequently, it should be suggested in the sense that it may be possible to obtain a new phase above 200 GPa.

To this end, all of the present work were carried out the first-principle calculation. It is reported to pay a special attention the predicted high-pressure phase with the P4/nmm structure which is predicted to be a semiconductor. We investigated the energy gap as a function of pressure by using the PBE, the mBJ, and the  $G_0W_0$  methods. As results, the calculations pointed out that three methods show a similar trend above a pressure of 190 GPa; however, it should note that the P4/nmm structure is still kept a semiconductor up to at least 190 GPa. Furthermore, the  $\text{HfO}_2$  that was investigated in this study would be superior to the metal-oxide-semiconductor devices of the next generation.

**Table 1.** Calculated energy gap of the HfO<sub>2</sub> in this work (at a pressure of 150 GPa) compared to previous calculations and experimental data.

Phase	method	Energy gap (eV)
P4/nmm-HfO <sub>2</sub>	GGA-PBE <sup>a</sup>	0.77
P4/nmm-HfO <sub>2</sub>	mBJ <sup>a</sup>	1.52
P4/nmm-HfO <sub>2</sub>	G <sub>0</sub> W <sub>0</sub> <sup>a</sup>	3.05
cubic-HfO <sub>2</sub>	GGA-PBE <sup>b</sup>	3.80
cubic-HfO <sub>2</sub>	HSE03 <sup>b</sup>	5.10
cubic-HfO <sub>2</sub>	HSE06 <sup>b</sup>	5.38
cubic-HfO <sub>2</sub>	PBE0 <sup>b</sup>	6.11
monoclinic-HfO <sub>2</sub>	Expt. <sup>c-f</sup>	5.7
cubic-HfO <sub>2</sub>	Expt. <sup>c-f</sup>	5.6–6
amorphous-HfO <sub>2</sub>	Expt. <sup>g,h</sup>	5.5

<sup>a</sup> This work.<sup>b</sup> Reference [51].<sup>c</sup> Reference [52].<sup>d</sup> Reference [53].<sup>e</sup> Reference [54].<sup>f</sup> Reference [55].<sup>g</sup> Reference [56].<sup>h</sup> Reference [57].

## 4. Conclusion

In summary, the structural behavior of HfO<sub>2</sub> under high pressure demonstrated the stable structures. High pressure phase of hafnium oxides HfO<sub>2</sub> is investigated and compared with those of hafnium and oxygen by using the first-principles calculations, based on the density functional theory, to examine the derived-ground state structure. The original hypothesis of the research, which is that HfO<sub>2</sub> will remain stable rather than decompose under the pressure of up to at least 200 GPa, was evidently confirmed. Our structural predictions have shown that a candidate high-pressure phase is found above 150 GPa: the tetragonal structure with the space group of P4/nmm, as its formation enthalpy lies on the Hf-O convex hull envelopes. HfO<sub>2</sub> displayed physical properties which can be categorized as semiconducting material by using the GGA-PBE method. Following this, the semiconductivity of the P4/nmm structure has been investigated theoretically, by considering the modified Becke-Johnson (mBJ) exchange potential formalism of the GGA functional and the GW approximation from 150 to 200 GPa. Moreover, the physical origin of semiconductor, based on the quasi-particle G<sub>0</sub>W<sub>0</sub>, manifested that the P4/nmm structure is likely to be metal at the pressure of 200 GPa. Our theoretical findings could pave the way for further studies to be conducted in metal oxides and suggests that hafnium oxide could be further investigated experimentally.

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## Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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