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A novel MgHe compound under high pressure

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Helium, with a full-shell electronic structure, is the most inert element in the periodic table at atmospheric pressure. The study of the reaction between helium and other non-noble-gas elements as well as relevant compounds has attracted great attention in the fields of chemistry, physics, materials and planetary science. In this study, we found a stable compound of MgHe with $P6_3/mmc$ symmetry at pressures above 795 GPa within zero-point energy. Thermodynamic stability calculations of $P6_3/mmc$ phase at high temperatures and pressures indicate that this structure may exist in the interior of the super-Earth and Neptune. Our further simulations on the electron localization function and Bader analysis show that the predicted compound is an electride with $-1.093e$ in the quantized interstitial quasiatom (ISQ) orbitals, which are localized at interstitial sites in the crystal lattice. Our study provides a theoretical basis for studying the physical and chemical properties of MgHe and the existence of MgHe in gaseous planets.

Keywords: high pressure, first-principles calculations, structure prediction

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1. Introduction

Helium is the second most abundant element in the universe after hydrogen with a mass fraction of ~ 23 wt%.[1,2] Therefore, the reaction between helium and other elements as well as the corresponding compounds is relevant to the chemistry and physics of planet science. On the other hand, magnesium, as one of the alkaline earth metals, is the ninth most abundant element in the universe,[3] and is the main component of the mantle in Earth-like planets and is a major part of the magnesium silicate that makes up the rocky core of the planet.[4–6] Therefore, the study of the reaction between helium and magnesium as well as the compounds formed is of fundamental interest for physics, chemistry and planet science.

It is well known that magnesium cannot react with helium and other noble gas elements at ambient, due to the robust stable electronic structure of noble gas elements. However, pressure has recently been found to activate this reaction, which is inaccessible under ambient conditions, since it can alter atomic distances and electronic structures. In previous studies, MgXe, Mg_2Xe and Mg_2Ar were predicted to become stable in a pressure range of 200–300 GPa, where magnesium obtains electrons from noble gas elements.[7] In addition, a series of helium-bearing compounds are predicted at high pressure.[8–21] To the best of our knowledge, there are no stable magnesium–helium compounds in previous theoretical and experimental studies. Helium is a major component of giant planet atmospheres and has been shown to exist inside giant planets.[22] Uranus and Neptune have stony cores and the main components of their cores are magnesium, magnesite, silica and magnesium iron silicate. The study of the interior composition of giant planets remains an important challenge in high-pressure science. Previous studies have reported that Si–O–H compounds[23] and Mg–O–H compounds[24] are probably components of the core–mantle boundary of giant planets. Therefore, it is necessary to study whether helium can react with magnesium to form new substances and can exist in the boundary of the core–mantle. Moreover, Na_2He was predicted to become stable at 113 GPa, where the electride feature of Na plays a key role in stabilizing this novel structure at high pressure.[17] At high pressure, magnesium is also found to exhibit an electride feature.[25] This motivates us to investigate whether Mg and He can form stable compounds and whether Mg–He compounds can exist in the interior of gaseous planets such as giant planets (Uranus and Neptune) and super-Earths.

In this study, we performed extensive structure searches for Mg–He systems in a pressure range of 500–1000 GPa. We evaluated the Gibbs free energy of Mg, He and MgHe to determine the phase stable range. The results show that MgHe is stable from 795–1000 GPa and 0–8000 K. An analysis of the electron localization function (ELF) and charge transfer in MgHe structure reveals that MgHe is an electride with electrons ($-1.093e$) localizing in the interatomic space.

2. Method

In order to research the stable structures of Mg_xHe_y ($x = y = 1, 2$) systems, the unbiased structure predictions

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were carried out using the CALYPSO code of the particle swarm optimization algorithm[26,27] at 500 GPa, 800 GPa and 1000 GPa with 1–8 molecular formula and 224 atoms. This method has proved to be very effective in finding new materials at high pressure.[28–30] For structural relaxations, we have used the Vienna *Ab initio* Simulation Package (VASP) code,[31,32] with the density functional theory (DFT),[33,34] the all-electron projector-augmented wave (PAW) method.[35] and the Perdew–Burke–Ernzerhof (PBE) parametrization.[36] For Mg and He elements, $2s^2 3s^2 3p^6$ and $1s^2$ were chosen as valence electrons. A plane-wave energy cutoff of 800 eV and a Monkhorst–Pack Brillouin sampling grid of $2\pi \times 0.03$ Å^{-1} were selected in our study.[37] In addition, the PHONOPY program is used to ensure the dynamic stability of the phase.[38,39]

To determine the phase boundaries between the solid phases, we have performed calculations to determine the Gibbs free energy $G(T,P) = \min_V[U(V) + PV + F_{\text{phonon}}(T,V)]$, where U, P, V and F_{phonon} are energy, pressure, volume and phonon free energy, respectively. The vibrational energy and entropy were obtained from lattice dynamic calculations using harmonic approximation as implemented in the PHONOPY code,

$$F_{\text{phonon}}(T,V) = k_{\text{B}}T \int_0^{\infty} g(\omega,V) \ln\left[2\sinh\left(\frac{\hbar\omega}{2k_{\text{B}}T}\right)\right] \mathrm{d}\omega,$$

where $g(\omega,V)$ is the phonon density of states at frequency ω and volume V. The minimal value of G was found at the equilibrium volume for a given T and P. Phonon calculations were carried out using a supercell approach as implemented in the PHONOPY code.[38]

The formation energies of Mg–He compounds with different compositions at 1 TPa and 0 K are shown in Fig. 1(a). The stable structures of magnesium element and helium corresponding to the pressure in our study have been previously reported. Helium is a hexagonal close-packed (hcp) structure at TPa.[40] Magnesium is in the fcc (*Fm*-3*m* phase) phase at 456 GPa and then transforms into the simple hexagonal (*P*6/*mmm* phase) phase at 756 GPa.[25,41–43] The MgHe compound on top of the convex hull is stable in contrast to other compositions, while Mg_2He and $MgHe_2$ compounds beyond the convex hull are not stable. The formation energy of MgHe compound with different pressure at 0 K is shown in Fig. 1(b). On this basis, MgHe compound has negative enthalpy of formation above 862 GPa without zero-point energy, indicating that it is stable above this pressure, although Mg_2He and $MgHe_2$ both have positive enthalpies in the 500–1000 GPa pressure range.

The MgHe compound is the only stable structure (Fig. 2(a)), and it crystalizes in a hexagonal structure (space group $P6_3/mmc$, 2 f.u. per cell) in a pressure range from 862 GPa to 1000 GPa. MgHe compound forms an anti-NiAs structure, in which He and Mg atoms are in an intercalated simple hexagonal lattice and a close-packed hexagonal structure. The lattice constants of $P6_3/mmc$ are $a = b = 2.280$ Å and $c = 2.682$ Å. The atomic position of Mg is 2*c* (0.333, 0.667, 0.250) and He is 2*a* (0, 0, 0.5). The coordination number (CN) of MgHe compound is 6. The distance of the closest He atom to magnesium is 1.478 Å. The Mg–Mg distance is 1.879 Å, shorter than twice the atomic radius of Mg (2.72 Å), but longer than the Mg–Mg distance in $P6/mmm$ phase of the Mg element at 1000 GPa. The insertion of helium atoms into the MgHe compound increases the distance between Mg and Mg atoms of $P6_3/mmc$ phase. We further checked phonon dispersions of MgHe $P6_3/mmc$ phase at 1000 GPa, and the results (Fig. 2(b)) show no imaginary frequencies in the whole Brillouin zone, meaning that they are dynamically stable at 1 TPa.

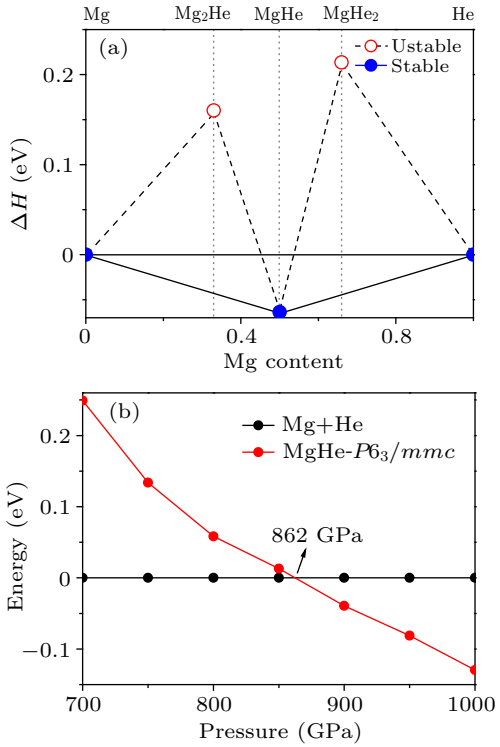


Fig. 1. The thermodynamic stability of Mg_xHe_y ($x = 1$, 2 and $y = 1$, 2) at 1 TPa and 0 K. (a) The thermodynamically stable compounds are marked as solid symbols, connected by a solid line. (b) The formation enthalpy of MgHe compound with respect to Mg + He from 700 GPa to 1000 GPa.

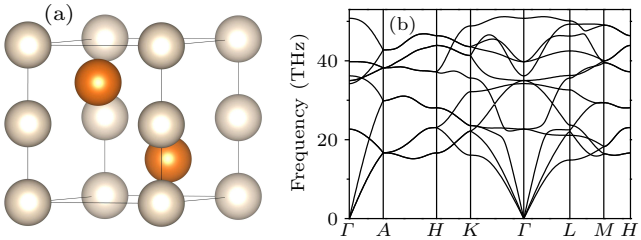


Fig. 2. Structural features and phonon dispersion curves of stable MgHe phases at 1 TPa. (a) $P6_3/mmc$ structure of MgHe at 1 TPa. (b) Phonon dispersion curves of $P6_3/mmc$ phase of MgHe at 1 TPa.

To find the reason for the stability of MgHe, we calcu-

lated and analyzed the change of formation enthalpy (ΔH), its energy components of internal energy (ΔE) and ΔPV term with increasing pressure. Learning from the Fig. 3, at lower pressures ($>$ 800 GPa), high enthalpy of MgHe compound is mainly caused by the high internal energy (ΔE). Above 800 GPa, the decrease formation enthalpy of MgHe is mainly due to the decrease in internal energy (ΔE). With the increase in pressure, the internal energy and volume of MgHe gradually decrease, and the formation energy (ΔH) of MgHe compound becomes negative at 862 GPa, thus becoming a stable compound, which is consistent with Fig. 1. The volume of MgHe compound is about 15% smaller than that of elemental Mg and helium at the initial stable pressure of 862 GPa. The bulk compression of some alkali metals and alkali metals under high pressure is due to the transfer of charge from the s orbital to the d orbital.[44] The reduction in the volume of MgHe is due to the charge of the 3s orbital of Mg transfer to the He or quantized interstitial quasiatom (ISQ) orbitals. The transfer of charge also causes a decrease in internal energy, especially under a pressure higher than 862 GPa.

The electron localization function (ELF)[45] is calculated to analyze the charge distribution and bonding characteristics of MgHe compound. As shown in Fig. 4(a), there is no charge distribution between the nearest Mg and He atoms meaning that MgHe compound has ionic properties. Mg–Xe and Mg–Ar compounds exhibit similar characteristics to MgHe in electronic structure and are ionic at lower pressures.[7] The local density function of MgHe shows that some electrons are localized in the interstitial position among Mg and He atoms and they do not belong to any atom. This electron property is the same as that of the high-pressure electride compound reported earlier.[46–48] This local electron density is formed due to the existence of quantized orbitals in the gap position limited by existing atoms. Since the orbital energy of ISQ varies by not more than the atomic orbital energy does with pressure, electrons will be moved from the atom to the ISQ orbital. MgHe is a high-pressure electride. However, MgAr and MgXe compounds are not electrides.[7]

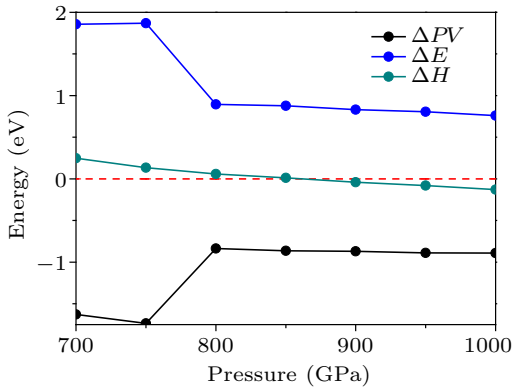


Fig. 3. Energy of MgHe compound under high pressure.

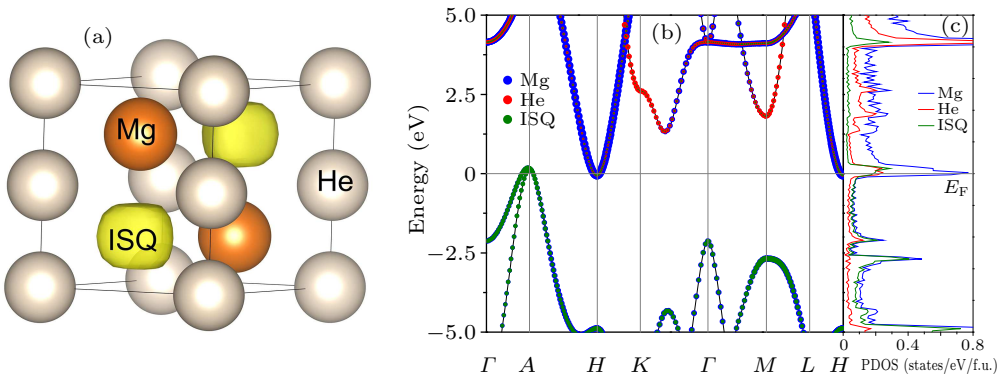


Fig. 4. Electronic structure of MgHe. (a) The electron localization functions of MgHe with $P6_3/mmc$ at 1 TPa. Iso-surface is 0.75. (b) Projected band-structure by element-weights of MgHe at 1 TPa in $P6_3/mmc$ phase. (c) Projected density of states of each element of MgHe at 1 TPa in $P6_3/mmc$ phase.

The projected band-structure and projected density of states (PDOS) of each element of $P6_3/mmc$ phase (Figs. 4(b)) and 4(c)) goes through the Fermi level at 1000 GPa, suggesting the metallic character of MgHe compound. According to the element weights from the projected band and the PDOS of each element, we reveal that the metal properties of MgHe are mainly contributed by the Mg element, while the contributions of helium and ISQ are similar, and their densities of states at Fermi energy are similar.

The Bader charge is also analyzed using Bader's quantum theory of atoms in molecules (QTAIM) approach[49] for MgHe compound under 1000 GPa, as shown in Table 1. Helium in MgHe compound has a $\sim -0.282e$ negative charge. He element in the known compounds He@H_2O, FeO_2He and Na_2He is $-0.03e$, $-0.04e$ and $-0.15e$, respectively. The Bader charge for Mg is close to $+1.375$, which is much smaller than that for the MgXe compound ($1.5e$) and MgO compound ($1.73e$) in typical rocksalt structure at 100 GPa. The large charge transfer for Mg indicated that the compound is strongly ionic with a strong Madelung field and an interstitially localized electron. The Bader charge of the ISQ of MgHe is $-1.093e$, which acts as an anion, and is much larger than the ISQ of Mg_2Xe electride of $-0.77e$. The charge transfer for both He and ISQ atoms comes from the Mg atoms in the

structure of $P6_3/mmc$ phase. This also proves that $P6_3/mmc$ Mg_2Xe is an electride, which is in agreement with the ELF calculation results. Simulations of the band of the MgHe stable compounds at 1000 GPa were performed to characterize the electronic properties (Figs. 4(b) and 4(c)). The band of $P6_3/mmc$ goes through the Fermi level at 1000 GPa, suggesting the metallic character of MgHe compound.

Table 1. The Bader charges of He, Mg and ISQ in $P6_3/mmc$ MgHe.

At 1 TPa	Mg	He	ISQ
$P6_3/mmc$	1.375	–0.282	–1.093

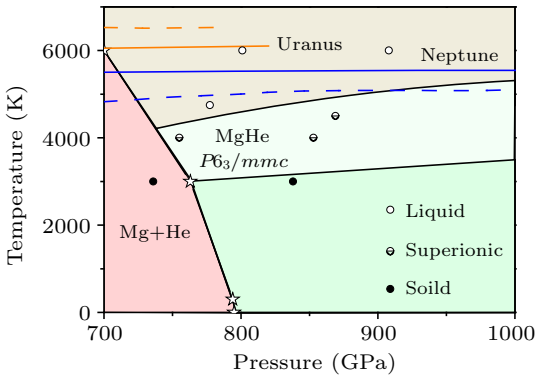


Fig. 5. The pressure temperature stability field of MgHe is relative to Mg and He elements. The solid black line plus five-star symbol is the decomposition curve. The part to the right of the decomposition curve represents the stable pressure and stable temperature region of MgHe-$P6_3/mmc$, and the left red part is the decomposition region of MgHe relative to Mg + He. The orange and blue solid and dash lines are two different models (U2 and N1)[50] of interior isentropic profiles of Uranus and Neptune, respectively. Different colored filled circles represent different states of the structure, with white representing the liquid state, semicircle representing the superionic state and black representing the solid state.

In order to study the high-temperature and high-pressure stability of MgHe compound, we constructed the P–T phase diagram of MgHe relative to He and Mg, as shown in Fig. 5. To determine the phase boundaries among the different phases, we calculated the Gibbs free energy. The vibrational energy and entropy were taken from lattice dynamic calculations through the quasi-harmonic approximation. Through molecular dynamics simulation, we obtained three different material states of MgHe: solid, liquid and superionic. Moreover, the stability intervals of MgHe in different material states are given by combining the temperature and pressure stability of MgHe compounds. The boundary between the liquid state and the superionic state is shown in Fig. 5, which is the melting curve of MgHe-$P6_3/mmc$ structure. According to the data in Fig. 5, as the pressure increases the stable temperature of MgHe decreases, which suggests that pressure increases the stable region of the MgHe compound. The zero-point energy (ZPE) reduces the lower stable pressure of the MgHe compound at the temperature of 0 K, which from 862 GPa without ZPE changes to 795 GPa within the ZPE. The isentropic profiles of Uranus and Neptune are within the stable pressure and temperature ranges of the new structures of MgHe compound that we have discovered. The Uranus and Neptune core–mantle boundaries are around 500–800 GPa and 5000–7000 K. The terrestrial planet (super-Earth) is equal to five Earth masses and its core–mantle boundary is about $\sim$ 600–700 GPa and $\sim$ 3000 K.[51,52] Therefore, comparing the temperature and pressure environment of the giant planet Neptune and super-Earth[50–52] and the stable range of the MgHe compound, we found that the stable temperature and pressure range of the $P6_3/mmc$ phase of MgHe overlaps with the temperature and pressure of the giant planet, suggesting that the $P6_3/mmc$ phase of MgHe may exist within the core–mantle boundary of giant planets or the mantle of super-Earths.

3. Conclusion

In this study, we predicted a new thermodynamically stable MgHe compound with $P6_3/mmc$ structure in the 795 GPa–1000 GPa pressure range. Band and Bader charge calculations show that it has ionic properties and weak metal properties. The electron localization function calculation indicates that it is an electride, and this structure has electrons localized at the interstitial position of the atom. The results of this study provide a theoretical basis for understanding the inert element compounds and electronic compounds. The comparison between the high-temperature and high-pressure stable range of MgHe compound and that of gaseous planets shows that MgHe compound may exist in the interior of giant planets and super-Earths, which provides a theoretical basis for studying the evolution of stars and the materials in the interior of stars.

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References

[1] Vopson M M 2021 *AIP Advances* **11** 105317
[2] Ezer D and Cameron A 1971 *Ap&SS* **14** 399
[3] Savage B D and Sembach K R 1996 *ARA&A* **34** 279
[4] Hubbard W, Nellis W, Mitchell A, Holmes N, Limaye S and McCandless P 1991 *Science* **253** 648
[5] Helled R, Anderson J D, Podolak M and Schubert G 2010 *Astrophys. J.* **726** 15
[6] MacFarlane J J and Hubbard W B 1982 *International Astronomical Union Colloquium* **60** 111
[7] Miao M S, Wang X L, Brgoch J, Spera F, Jackson M G, Kresse G and Lin H Q 2015 *J. Am. Chem. Soc.* **137** 14122
[8] Loubeyre P, Jean-Louis M, LeToullec R and Charon-Gérard L 1993 *Phys. Rev. Lett.* **70** 178

[9] Gao H, Sun J, Pickard C J and Needs R J 2019 *Phys. Rev. Mater.* **3** 015002
[10] Plisson T, Weck G and Loubeyre P 2014 *Phys. Rev. Lett.* **113** 025702
[11] Kooi M and Schouten J 1999 *Phys. Rev. B* **60** 12635
[12] Yu X, Zhu J, Du S, Xu H, Vogel S C, Han J, Germann T C, Zhang J, Jin C and Francisco J S 2014 *Proc. Natl. Acad. Sci. USA* **111** 10456
[13] Dyadin Y A, Larionov É G, Aladko E Y, Manakov A Y, Zhurko F V, Mikina T V, Komarov V Y and Grachev E V 1999 *J. Struct. Chem.* **40** 790
[14] Teeratchanan P and Hermann A 2015 *J. Chem. Phys.* **143** 154507
[15] Liu H, Yao Y and Klug D D 2015 *Phys. Rev. B* **91** 014102
[16] Teeratchanan P and Hermann A 2015 *J. Chem. Phys.* **143** 154507
[17] Dong X, Oganov A R, Goncharov A F, Stavrou E, Lobanov S, Saleh G, Qian G R, Zhu Q, Gatti C and Deringer V L 2017 *Nat. Chem.* **9** 440
[18] Liu Z, Botana J, Hermann A, Valdez S, Zurek E, Yan D, Lin H Q and Miao M S 2018 *Nat. Commun.* **9** 4383
[19] Ninet S, Weck G, Loubeyre P and Datchi F 2011 *Phys. Rev. B.* **83** 134107
[20] Vos W, Finger L, Hemley R, Hu J, Mao H and Schouten J 1992 *Nature* **358** 46
[21] Li Y, Feng X, Liu H, Hao J, Redfern S A, Lei W, Liu D and Ma Y 2018 *Nat. Commun.* **9** 722
[22] Shi J, Cui W, Hao J, Xu M, Wang X and Li Y 2020 *Nat. Commun.* **11** 1
[23] Gao H, Liu C, Shi J, Pan S, Huang T, Lu X, Wang H T, Xing D and Sun J 2022 *Phys. Rev. Lett.* **128** 035702
[24] Pan S, Huang T, Vazan A, Liang Z, Liu C, Wang J, Pickard C J, Wang H T, Xing D and Sun J 2023 *Nat. Commun.* **14** 1165
[25] Li P, Gao G, Wang Y and Ma Y 2010 *J. Phys. Chem. C* **114** 21745
[26] Wang Y, Lv J, Zhu L and Ma Y 2010 *Phys. Rev. B.* **82** 094116
[27] Wang Y, Lv J, Zhu L and Ma Y 2012 *Comput. Phys. Commun.* **183** 2063
[28] Zhang J, Liu H, Ma Y and Chen C 2022 *Natl. Sci. Rev.* **9** nwab168
[29] Zhong X, Sun Y, Iitaka T, Xu M, Liu H, Hemley R J, Chen C and Ma Y 2022 *J. Am. Chem. Soc.* **144** 13394
[30] Zhu L, Liu H, Pickard C J, Zou G and Ma Y 2014 *Nat. Chem.* **6** 644
[31] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865
[32] Kresse G and Furthmüller J 1996 *Phys. Rev. B.* **54** 11169
[33] Kohn W and Sham L J 1965 *Phys. Rev.* **140** A1133
[34] Hohenberg P and Kohn W 1964 *Phys. Rev.* **136** B864
[35] Kresse G and Joubert D 1999 *Phys. Rev. B* **59** 1758
[36] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865
[37] Zhong X, Li X, Yang L, Wang D, Qu X and Liu H 2021 *J. Phys. Chem. Lett.* **12** 1671
[38] Togo A, Oba F and Tanaka I 2008 *Phys. Rev. B* **78** 134106
[39] Baroni S, Giannozzi P and Testa A 1987 *Phys. Rev. Lett.* **58** 1861
[40] Monserrat B, Drummond N D, Pickard C J and Needs R J 2014 *Phys. Rev. Lett.* **112** 055504
[41] Zhu Q, Oganov A R and Lyakhov A O 2013 *PCCP* **15** 7696
[42] McMahan A and Moriarty J A 1983 *Phys. Rev. B* **27** 3235
[43] Stinton G W, MacLeod S G, Cynn H, Errandonea D, Evans W J, Proctor J E, Meng Y and McMahon M I 2014 *Phys. Rev. B.* **90** 134105
[44] Takemura K, Minomura S and Shimomura O 1982 *Phys. Rev. Lett.* **49** 1772
[45] Silvi B and Savin A 1994 *Nature* **371** 683
[46] Ma Y, Eremets M, Oganov A R, Xie Y, Trojan I, Medvedev S, Lyakhov A O, Valle M and Prakapenka V 2009 *Nature* **458** 182
[47] Lv J, Wang Y, Zhu L and Ma Y 2011 *Phys. Rev. Lett.* **106** 015503
[48] Marqués M, Ackland G, Lundegaard L, Stinton G, Nelmes R, McMahon M and Contreras-García J 2009 *Phys. Rev. Lett.* **103** 115501
[49] Bader R F 1985 *Acc. Chem. Res.* **18** 9
[50] Nettelmann N, Helled R, Fortney J and Redmer R 2013 *Planet. Space Sci.* **77** 143
[51] McWilliams R S, Spaulding D K, Eggert J H, Celliers P M, Hicks D G, Smith R F, Collins G W and Jeanloz R 2012 *Science* **338** 1330
[52] Valencia D, O'Connell R J and Sasselov D 2006 *Icar* **181** 545