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SPECIAL TOPIC — Structures and properties of materials under high pressure

Pressure-driven crystal structure evolution in RbB_2C_4 compounds

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As an extreme physical condition, high pressure serves as a potent means to substantially modify the interatomic distances and bonding patterns within condensed matter, thereby enabling the macroscopic manipulation of material properties. We employed the CALYPSO method to predict the stable structures of RbB_2C_4 across the pressure range from 0 GPa to 100 GPa and investigated its physical properties through first-principles calculations. Specially, we found four novel structures, namely, $P6_3/mcm$-, $Amm2$-, $P1$-, and $I4/mmm$-RbB_2C_4. Under pressure conditions, electronic structure calculations reveal that all of them exhibit metallic characteristics. The calculation results of formation enthalpy show that the $P6_3/mcm$ structure can be synthesized within the pressure range of 0–40 GPa. Specially, the $Amm2$, $P1$, and $I4/mmm$ structures can be synthesized above 4 GPa, 6 GPa, 10 GPa, respectively. Moreover, the estimated Vickers hardness value of $I4/mmm$-RbB_2C_4 compound is 47 GPa, suggesting that it is a superhard material. Interestingly, this study uncovers the continuous transformation of the crystal structure of RbB_2C_4 from a layered configuration to folded and tubular forms, ultimately attaining a stabilized cage-like structure under the pressure span of 0–100 GPa. The application of pressure offers a formidable impetus for the advancement and innovation in condensed matter physics, facilitating the exploration of novel states and functions of matter.

Keywords: first-principles calculation, high pressure, RbB_2C_4 compounds, crystal structure prediction

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1. Introduction

The discovery of new materials is of great significance for the progress of industry. The synthesis of new materials can be accomplished either by precisely regulating the key parameters involved in the process or by adjusting the external factors that have an impact on the materials.[1–5] Pressure is one of the fundamental thermodynamic variables, which can allow precisely tuning of the interatomic distance and alter the bonding patterns of materials, leading to phase transformations into high-pressure structures with unusual chemical and physical properties.[6–18]

In recent years, advances in experimental and theoretical techniques have fostered remarkable breakthroughs in high-pressure science, as exemplified by the discovery of high-pressure superconductors, metal-to-semiconductor transitions, superfluids, etc.[19–22] It is noteworthy that Zhu *et al*. employed the CALYPSO (Crystal structure AnaLYsis by Particle Swarm Optimization) method to make predictions and subsequently succeeded in synthesizing the SrB_3C_3 compound under a pressure of approximately 50 GPa.[23] Further calculations show that SrB_3C_3 is a superconductor with a superconducting critical temperature of about 40 K.[24–27] In addition, the physical properties of various boron–carbon compounds doped with different elements have been investigated under high pressure, such as SrB_2C_4, BaB_2C_4, $Na_2B_4C_8$, $Li_2B_4C_8$ and so on.[28–31] Since Sr and Rb are located in the same period of the periodic table, they exhibit similar chemical and physical properties. This prompted us to systematically explore the crystal structure characteristics of RbB_2C_4 in the pressure range of 0–100 GPa.

In this work, we used the CALYPSO method to predict the crystal structure of RbB_2C_4 in the pressure range of 0–100 GPa, and studied its physical properties by first-principles calculations. We found that the crystal structure of RbB_2C_4 has undergone a continuous evolution process from layered to folded, then to tubular, and finally is stabilized into a clathrate structure in the pressure range of 0–100 GPa. Under pressure condition, electronic structure calculations reveal that all of them exhibit metallic characteristics. Moreover, the estimated Vickers hardness value of $I4/mmm$-RbB_2C_4 compound is 47 GPa, suggesting that it is a superhard material. The introduction of pressure provides a powerful driving force for the development and innovation of condensed matter physics, facilitating the exploration of novel states and functions of matter.

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2. Computational methods

We explored the crystal structures of RbB_2C_4 under pressure by using the software package CALYPSO, which can predict crystal structures that are energetically stable or metastable under the given pressure condition and chemical composition.[32–36] First-principles electronic structure calculations were based on density functional theory (DFT) and performed using the Vienna *ab initio* simulation package (VASP).[37,38] The Perdew–Burke–Ernzerhof (PBE) parametrization of the generalized gradient approximation (GGA) was used.[39,40] We used projector augmented wave (PAW) potentials in which the valence electrons for the Rb, B, and C atoms were represented as $4s^2 4p^6 5s^1$, $2s^2 2p^1$, and $2s^2 2p^2$, respectively.[41] For the lowest energy structure, we used 800 eV energy truncation and high-density Monkhorst–Pack k point grid for more detailed calculations.[42] This is done to ensure that the total energy can reach a convergence accuracy of about 1 meV/atom during the structural optimization process. The dynamic stability of the predicted structure is determined by the phonon dispersion curves using the supercell method implemented in PHONOPY program.[43] The Vickers hardness values are estimated by using the microscopic hardness model.[44–47]

3. Results and discussion

We predict the crystal structure of RbB_2C_4 compound in the pressure range of 0–100 GPa, and propose four new structures, namely, $P6_3/mcm$-, $Amm2$-, $P1$-, and $I4/mmm$-RbB_2C_4. The pressure–composition phase diagram of the RbB_2C_4 compounds is shown in Fig. 1(a), which expresses the pressure interval for the existence of different phases. Within the pressure range from 0 GPa to 15 GPa, the $P6_3/mcm$ phase exhibits the lowest energy and thus predominates. Once the pressure exceeds 15 GPa, the $Amm2$ phase becomes more thermodynamically stable. As the pressure further increases to 40 GPa, a transformation into a novel triclinic $P1$ phase takes place. Eventually, when the pressure attains 72 GPa, the $I4/mmm$ phase emerges as the most energetically favorable and stable configuration. The structures are shown in Figs. 1(b)–1(e). The $P6_3/mcm$-RbB_2C_4 at ambient pressure has a layered hexagonal structure, separated by a B–C honeycomb layer and interstitial Rb atoms. The bond length between boron and carbon is 1.552 Å, and the bond length between carbon and carbon is 1.455 Å. In the $Amm2$-RbB_2C_4 structure, boron and carbon atoms form a complex network structure, which consists of folded six-membered ring and three-membered ring. These boron–carbon network structures are separated by the Rb atomic layer. The boron–carbon bond of the $P1$-RbB_2C_4 is tubular and the rubidium atom is located at the centre of the tube. The $I4/mmm$-RbB_2C_4 has a sodalite-like clathrate structure, which is composed of six square surfaces and eight hexagonal surfaces, in which rubidium atoms occupy the central position of the clathrate structure. In the pressure range of 0–100 GPa, the crystal structure of RbB_2C_4 has undergone a continuous evolution process from layer to fold, and is finally stabilized to clathrate. Our study has found the evolution of crystal structure under pressure, which provides a theoretical basis for the stability and phase transition of crystal structure under normal pressure and high pressure.

Furthermore, we calculated the formation enthalpies of the RbB_2C_4 compounds with respect to pressure via two possible synthetic pathways. The formation enthalpy for RbB_2C_4 is defined as

$$\Delta H = H(RbB_2C_4) - H(Rb) - \frac{4}{3}H(\text{h-}BC_3) - \frac{2}{3}H(B), \quad (1)$$

$$\Delta H = H(RbB_2C_4) - H(Rb) - \frac{4}{3}H(\text{g-}BC_3) - \frac{2}{3}H(B). \quad (2)$$

For the Rb atom, we used the enthalpy from $bcc \rightarrow fcc \rightarrow I4_1/amd \rightarrow Cmca$ structure transitions, with the phase transitions occurring at 8 GPa, 15 GPa and 41 GPa, respectively.[48] For the B atom, we used the enthalpy from $R\bar{3}m \rightarrow Pnnm(\gamma\text{-}B) \rightarrow Cmca(\alpha\text{-}Ga)$ structure transitions, with the phase transitions occurring at 18 GPa and 91 GPa, respectively.[49] For BC_3, we used h-BC_3 in the calculation.[50,51] As shown in Fig. 2(a), when h-BC_3 serves as the precursor, the calculated results indicate that the $Amm2$, $P1$, and $I4/mmm$ structures can be synthesized at pressures above 4 GPa, 6 GPa and 10 GPa, respectively. As shown in Fig. 2(b), when g-BC_3 is utilized as the precursor, the calculation results revealed that the synthesis of these three structures necessitates pressures above 8 GPa, 10 GPa and 16 GPa, respectively. Therefore, it can be concluded that the employment of h-BC_3 as a precursor entails a lower synthesis pressure compared to that of g-BC_3.

We calculated phonon dispersion curves for $P6_3/mcm$ at 0 GPa and 10 GPa, for $Amm2$ at 0 GPa and 40 GPa, for $P1$ at 0 GPa and 70 GPa, and for $I4/mmm$ at 0 GPa and 100 GPa, as shown in Fig. 3. At both 0 GPa and 10 GPa, the $P6_3/mcm$ structure displays imaginary frequencies specifically within the regions from Γ to A, K to Γ, and Γ to M in the Brillouin zone. In these particular regions of reciprocal space, the dynamic stability of the Rb atomic layer is unstable. From the phonon spectrum of the $Amm2$ phase, it can be observed that an imaginary frequency exists within the Brillouin zone at 0 GPa, indicating that the structure is dynamically unstable at ambient pressure. Nevertheless, when the pressure is increased to 40 GPa, no imaginary frequency is observed in the phonon spectrum, which indicates that the dynamic properties of the $Amm2$ phase are stable under this pressure. Under ambient pressure and corresponding high-pressure conditions, the $P1$ and $I4/mmm$ phases have no imaginary frequencies in the entire Brillouin zone, which indicates that these phases are dynamically stable within the pressure range studied.

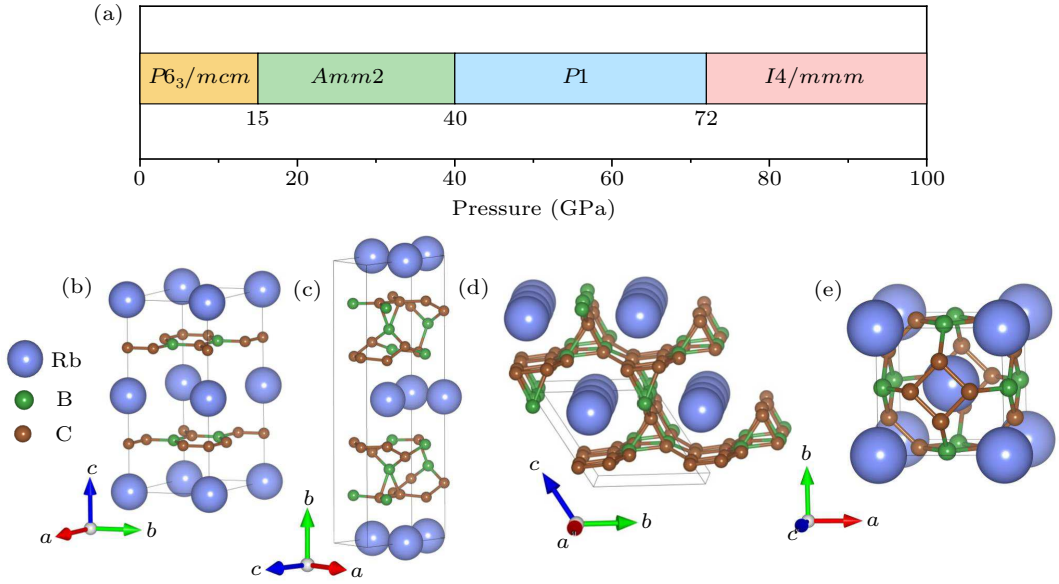


Fig. 1. (a) Phase diagram of the RbB_2C_4 compounds under high pressures. Crystal structures of (b) $P6_3/mcm$-, (c) $Amm2$-, (d) $P1$-, (e) $I4/mmm$-RbB_2C_4.

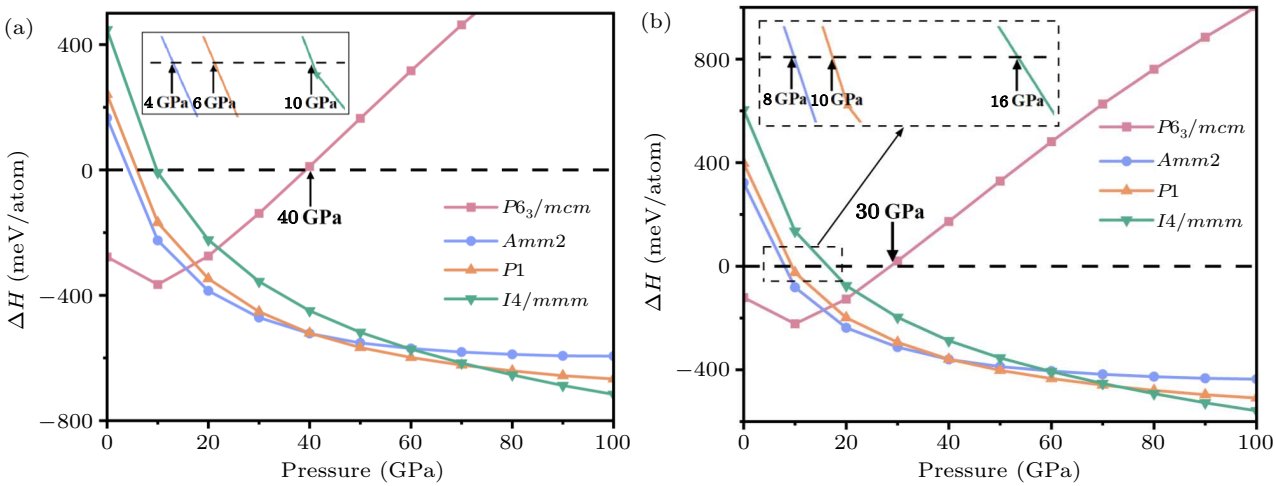


Fig. 2. The formation enthalpies of the $P6_3/mcm$, $Amm2$, $P1$ and $I4/mmm$ structures along two different paths.

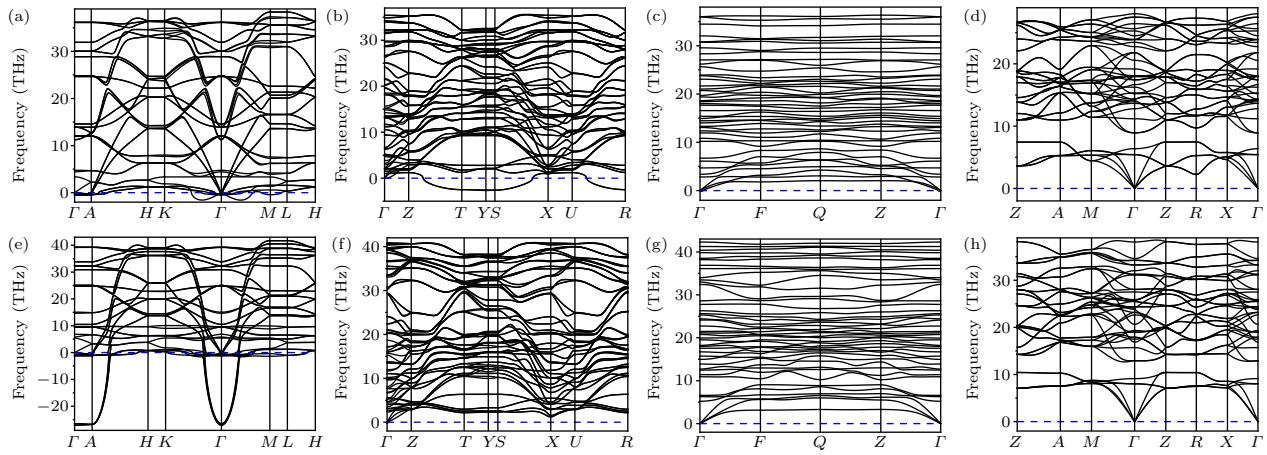


Fig. 3. Calculated phonon dispersion curves for (a) $P6_3/mcm$ at 0 GPa, (b) $Amm2$ at 0 GPa, (c) $P1$ at 0 GPa, (d) $I4/mmm$ at 0 GPa, (e) $P6_3/mcm$ at 10 GPa, (f) $Amm2$ at 40 GPa, (g) $P1$ at 70 GPa, (h) $I4/mmm$ at 100 GPa.

We next explored the electronic properties of the predicted RbB_2C_4 compounds via electronic band structures and densities of electronic states (DOSs). We studied the electronic properties of these compounds by calculating the band structure and the density of states. As shown in Fig. 4, it can be clearly seen from the energy band diagram that it

passes through the vicinity of the Fermi surface, indicating that the electronic properties of these compounds exhibit metallic characteristics. It can be observed that there is a significant consistency between the band structures and DOS. In addition, the major contribution of metallicity comes from the B-p state and the C-p state.

We investigated the mechanical properties of the RbB_2C_4 compounds. The elastic constants of stable orthorhombic compounds need to satisfy $C_{11} > 0$, $C_{11}C_{22} > C_{12}^2$, $(C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2) > 0$, $C_{44} > 0$, $C_{55} > 0$ and $C_{66} > 0$; the elastic constant of stable tetragonal compounds need to satisfy $C_{11} > 0$, $C_{33} > 0$, $C_{44} > 0$, $C_{66} > 0$, $(C_{11} - C_{12}) > 0$, $(C_{11} + C_{33} - 2C_{13}) > 0$ and $[2(C_{11} + C_{12}) + C_{33} + 4C_{13}] > 0$. We further calculated the elastic constants, bulk modulus, shear modulus, Poisson's ratio and hardness values, as shown in Table 1. The results calculated according to the mechanical stability standard show that only the *Amm*2 and *I*4/*mmm* phases are mechanically stable under ambient pressure. The shear modulus, bulk moduli, and Vickers hardness were computed by using the H_v^{Chen} and H_v^{Tian} models for hardness.[44–47] According to the calculation results in Table 1, the H_v^{Chen} values of *Amm*2-RbB_2C_4 and *I*4/*mmm*-RbB_2C_4 are 29 GPa and 47 GPa, respectively, indicating that the *Amm*2 structure is a hard material, and the *I*4/*mmm* structure is a superhard material.

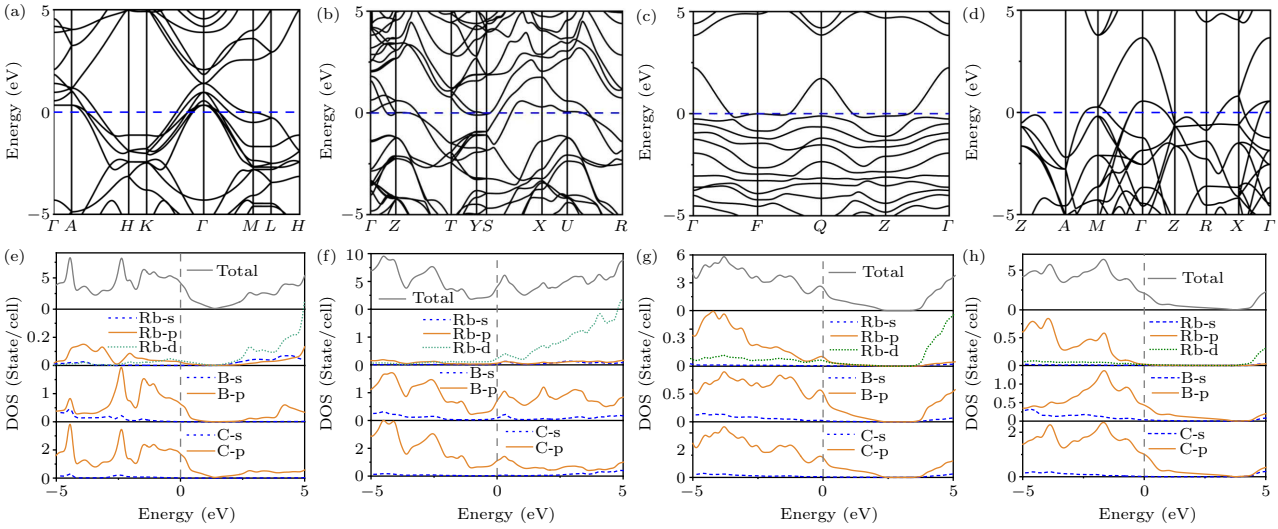


Fig. 4. Electronic band structures and density of states of (a) and (e) *P*6$_3$/*mcm* at 10 GPa, (b) and (f) *Amm*2 at 40 GPa, (e) and (g) *P*1 at 70 GPa, (d) and (h) *I*4/*mmm* at 100 GPa.

Table 1. Calculated elastic constants C_{ij}, bulk modulus B, shear modulus G, and Vickers hardness H_v (all in units of GPa) of RbB_2C_4 at 0 GPa.

Space group	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	B	G	G/B	H_v^{Chen}	H_v^{Tian}
Diamond	1046			564			128		434	519	0.84	93	94
c-BN	776			445			171		373	381	0.98	63	63
*Amm*2	698	293	523	112	186	96	31	44	186	158	0.85	29	27
*I*4/*mmm*	547	575	480	224	224	234	74	66	226	231	1.02	47	45

4. Conclusion

In summary, we have extensively explored the RbB_2C_4 within the pressure range of 0–100 GPa using CALYPSO method and proposed four new structures of *P*6$_3$/*mcm*-, *Amm*2-, *P*1-, and *I*4/*mmm*-RbB_2C_4. We found that the crystal structure of RbB_2C_4 gradually evolved from layered to folded, then to tubular, and finally to clathrate structure in the pressure range of 0–100 GPa. The calculation results of formation enthalpy show that the *P*6$_3$/*mcm* structure can be synthesized in the range of 0–40 GPa; *Amm*2, *P*1, and *I*4/*mmm* structures can be synthesized above 4 GPa, 6 GPa, 10 GPa, respectively. The electronic band structures and densities of electronic states suggest that these compounds exhibit metallic characteristics. The calculation results of Vickers hardness show that the *I*4/*mmm* clathrate structure exhibits superhard characteristics. This research uncovers the transformation process of the crystal structure of the RbB_2C_4 compound with the increase of pressure. Such a discovery injects novel theoretical perspectives into the domain of high-pressure-induced crystal structure phase transitions, thereby enriching the existing knowledge reservoir and potentially inspiring further investigations and advancements in this area of study.

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References

[1] Holzapfel W B 1996 *Reports on Progress in Physics* **59** 29
[2] Mujica A, Rubio A, Muñoz A and Needs R J 2003 *Rev. Mod. Phys.* **75** 863
[3] Degtyareva O, MCMahon M I and Nelmes R J 2004 *High Press Res.* **24** 319
[4] Xia H, Parthasarathy G, Luo H, Vohra Y K and Ruoff A L 1990 *Phys. Rev. B* **42** 6736
[5] Xia H, Duclos S J, Ruoff A L and Vohra Y K 1990 *Phys. Rev. Lett.* **64** 204
[6] Zhu L, Wang Z, Wang Y, Zou G, Mao H and Ma Y 2012 *Proc. Natl. Acad. Sci. USA* **109** 751
[7] Mao H and Hemley R J 1994 *Rev. Mod. Phys.* **66** 671
[8] McMahon M I, Gregoryanz E, Lundegaard L F, Loa I, Guillaume C, Nelmes R J, Kleppe A K, Amboage M, Wilhelm H and Jephcoat A P 2007 *Proc. Natl. Acad. Sci. USA* **104** 17297
[9] Tse J S, Desgreniers S, Ohishi Y and Matsuoka T 2012 *Sci. Rep.* **2** 372
[10] Ma Y, Tse J S and Klug D D 2003 *Phys. Rev. B* **67** 140301
[11] Eremets M I, Gavriliuk A G, Trojan I A, Dzivenko D A and Boehler R 2004 *Nat. Mater.* **3** 558
[12] Khaliullin R Z, Eshet H, Kühne T D, Behler J and Parrinello M 2011 *Nat. Mater.* **10** 693
[13] Fujii Y, Hase K, Ohishi Y, Fujihisa H, Hamaya N, Takemura K, Shimomura O, Kikegawa T, Amemiya Y and Matsushita T 1989 *Phys. Rev. Lett.* **63** 536
[14] Gregoryanz E, Lundegaard L F, McMahon M I, Guillaume C, Nelmes R J and Mezouar M 2008 *Science* **320** 1054
[15] Gregoryanz E, Degtyareva O, Somayazulu M, Hemley R J and Mao H 2005 *Phys. Rev. Lett.* **94** 185502
[16] Kim E and Chan M H W 2006 *Phys. Rev. Lett.* **97** 115302
[17] Shimizu K, Suhara K, Ikumo M, Eremets M I and Amaya K 1998 *Nature* **393** 767
[18] Gao G, Oganov A R, Bergara A, Martinez-Canales M, Cui T, Iitaka T, Ma Y and Zou G 2008 *Phys. Rev. Lett.* **101** 107002
[19] Chang K J, Dacorogna M M, Cohen M L, Mignot J M, Chouteau G and Martinez G 1985 *Phys. Rev. Lett.* **54** 2375
[20] 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
[21] Matsuoka T and Shimizu K 2009 *Nature* **458** 186
[22] Babaev E, Sudbø A and Ashcroft N W 2004 *Nature* **431** 666
[23] Zhu L, Strobel T A and Cohen R E 2020 *Phys. Rev. Lett.* **125** 127601
[24] Zhu L, Liu H, Somayazulu M, Meng Y, Guńka P A, Shiell T B, Kenney-Benson C, Chariton S, Prakapenka V B, Yoon H, Horn J A, Paglione J, Hoffmann R, Cohen R E and Strobel T A 2023 *Phys. Rev. Res.* **5** 013012
[25] Wang J N, Yan X W and Gao M 2021 *Phys. Rev. B* **103** 144515
[26] Gai T T, Guo P J, Yang H C, Gao Y, Gao M and Lu Z Y 2022 *Phys. Rev. B* **105** 224514
[27] Zhang P, Li X, Yang X, Wang H, Yao Y and Liu H 2022 *Phys. Rev. B* **105** 094503
[28] Cui Z, Zhang X, Sun Y, Liu Y and Yang G 2022 *Phys. Chem. Chem. Phys.* **24** 16884
[29] Liu A, Cheng X, Wang X, Zou Y and Zhang M 2023 *Phys. Chem. Chem. Phys.* **25** 20837
[30] Cheng X, Liu A, Wang X, Zou Y, Zhang M and Gao L 2023 *J. Alloys Compd.* **969** 172466
[31] Fang C M, Bauer J, Saillard J Y and Halet J F 2007 *J. Solid State Chem.* **180** 2465
[32] Yan H, Chen L, Wei Z, Zhang M and Wei Q 2020 *Vacuum* **180** 109617
[33] Lazicki A, Yoo C S, Cynn H, Evans W J, Pickett W E, Olamit J, Liu K and Ohishi Y 2007 *Phys. Rev. B* **75** 054507
[34] Wang Y, Lv J, Zhu L and Ma Y 2012 *Comput. Phys. Commun.* **183** 2063
[35] Wang Y, Lv J, Zhu L and Ma Y 2010 *Phys. Rev. B* **82** 094116
[36] Gao B, Gao P, Lu S, Lv J, Wang Y and Ma Y 2019 *Sci. Bull.* **64** 301
[37] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865
[38] Perdew J P and Wang Y 1992 *Phys. Rev. B* **45** 13244
[39] Hohenberg P and Kohn W 1964 *Phys. Rev.* **136** B864
[40] Kohn W and Sham L J 1965 *Phys. Rev.* **140** A1133
[41] Kresse G and Joubert D 1999 *Phys. Rev. B* **59** 1758
[42] Monkhorst H J and Pack J D 1976 *Phys. Rev. B* **13** 5188
[43] Togo A and Tanaka I 2015 *Scr. Mater.* **108** 1
[44] Chen X Q, Niu H, Li D and Li Y 2011 *Intermetallics* **19** 1275
[45] Chen X Q, Niu H, Franchini C, Li D and Li Y 2011 *Phys. Rev. B* **84** 121405
[46] Tian Y, Xu B and Zhao Z 2012 *Int J. Refract Metals Hard Mater* **33** 93
[47] Mouhat F and Coudert F X 2014 *Phys. Rev. B* **90** 224104
[48] Degtyareva O 2010 *High Press Res.* **30** 343
[49] Oganov A R, Solozhenko V L, Gatti C, Kurakevych O O and Le Godec Y 2012 *J. Superhard Mater.* **34** 74
[50] Kharabadze S, Meyers M, Tomassetti C R, Margine E R, Mazin I I and Kolmogorov A N 2023 *Phys. Chem. Chem. Phys.* **25** 7344
[51] Milashius V, Pavlyuk V, Dmytriv G and Ehrenberg H 2018 *Inorg. Chem. Front.* **5** 853