In this paper, we systematically investigated the structural and magnetic properties of CrTe by combining particle swarm optimization algorithm and first-principles calculations. By considering the electronic correlation effect, we predicted the ground-state structure of CrTe to be NiAs-type (space group $P6_3/mmc$) structure at ambient pressure, consistent with the experimental observation. Moreover, we found two extra meta-stable $Cmca$ and $R3m$ structures which have negative formation enthalpy and stable phonon dispersion at ambient pressure. The $Cmca$ structure is a layered antiferromagnetic metal. The cleaved energy of a single layer is 0.464 J/m$^2$, indicating the possible synthesis of CrTe monolayer. The $R3m$ structure is a ferromagnetic half-metal. When external pressure is applied, the ground-state structure of CrTe transitions from $P6_3/mmc$ structure to $R3m$ structure at a pressure of 34 GPa, then to $Fm\bar{3}m$ structure at 42 GPa. We thought these results help to motivate experimental studies of the CrTe compounds in the application of spintronics.

Keywords CrTe, meta-stable structure, antiferromagnetic metal, ferromagnetic half-metal
where \( 2 \) is the number of atoms per CrTe formula. The

When the external pressure increased, the ground-state structure of CrTe changes from FM half-metal. Their electronic and magnetic properties were carefully analyzed. When the external pressure increases, the ground-state structure of CrTe changes from \( P6_3/mmc \) to \( R\bar{3}m \) at 34 GPa, and then to \( Fm\bar{3}m \) structure at 42 GPa.

### 2 Methods of computational

The searching of crystal structure was performed by particle swarm optimization algorithm, as implemented in the CALYPSO code [23–25]. Given the chemical composition and external pressure, the atomic arrangement with the global lowest energy on the potential energy surface can be determined [26, 27]. This algorithm has been applied to many systems with reliability [26, 27]. We searched for the low-energy structures of bulk (CrTe)\(_n\) with number of formula \( n \) from 1 to 4 in the process of the structure prediction. To judge the stability of the CrTe in various structures, we adopted the formation enthalpy (\( \Delta H \)) that is defined as

\[
\Delta H = [h(\text{CrTe}) - h(\text{Cr}) - h(\text{Te})]/2, \tag{1}
\]

where \( 2 \) is the number of atoms per CrTe formula. The \( h(\text{CrTe}) \) is the enthalpies per formula corresponding to the most stable magnetic state of CrTe. \( h(\text{Cr}) \) and \( h(\text{Te}) \) are the enthalpy of Cr substance (space group Im\(\bar{3}m \)) [28] and Te substance (space group \( P3_121 \)) [29], respectively. The first-principles calculations were performed using the Vienna ab initio simulation package (VASP) [30, 31]. The projector augmented wave (PAW) [32] pseudopotentials and Perdew, Burke, and Ernzerhof (PBE) [33] exchange-correlation functionals were used. A plane-wave basis set with an energy cutoff of 500 eV and a Monkhorst-Pack [34] k-points with a grid spacing of \( 2\pi \times 0.08 \text{ Å}^{-1} \) were used. The crystal structures and atomic positions were fully optimized with a force convergence threshold of 0.01 eV/Å. To consider the correlation effects of Cr-d orbitals, we applied the PBE+U scheme [35]. The onsite effective \( U_f \) value of Cr-d electrons in CrTe system was determined to be 4 eV (see Fig. S1) by the linear response methods [36]. The phonon spectrum was calculated using density functional perturbation theory [37].

### 3 Results and discussion

#### 3.1 Meta-stable structures

Calculated formation enthalpies of CrTe compounds, within the chemical compositions available in the experiment [9–14], show that Cr–Te compound with a Cr:Te ratio of 1:1 has the lowest formation enthalpy \( \Delta H \) (see Fig. S9). Through the structural search at ambient pressure, several structures in CrTe system with a large negative \( \Delta H \) including \( Cmca, P6_3/mmc \) (NA), \( R\bar{3}m \) and \( Fm\bar{3}m \) (RS) structures are predicted (see Fig. 1), while the ZB and MnP structures have much smaller negative \( \Delta H \). The energy-volume curve of four low-energy structures are displayed in Fig. 2. Considering the layered structure of the \( Cmca \) phase, we adopted the van der Waals (vdw) functional [38] in the first-principles calculations. In PBE calculations, the \( Cmca \) structure is the ground-state structure and \( P6_3/mmc \) structure is a meta-
stable one [see Fig. 2(a)]. However, in PBE+U calculations, the \( \text{P6}_{3} / \text{mmc} \) (\( \text{NA} \)) structure becomes the ground-state structure [see Fig. 2(b)] which is consistent with the available experiments [9, 10]. It was indicated that the electronic correlation effect has to be considered in the investigation of the structures of CrTe. Our results about the ground state of CrTe in PBE and PBE+U calculations are different from previous works [15, 17, 20–22] (see Table S1). Firstly, both the \( \text{Cmca} \) and \( \text{R3m} \) phases have not been considered in previous works. Secondly, the FP-LAPWs method and MBJ method [15, 20–22] may not be suited for determining the ground state of CrTe. For example, the FP-LAPW method can not calculate stress tensor, which makes the optimization tedious for low symmetry cases [39]. On the other side, the MBJ method is a potential-only functional and is not suited for computing Hellmann–Feynman forces [40]. In the following content, we will display the results of PBE+U calculations.

The optimized lattice parameters of low-energy CrTe structures are given in Table 1. The phonon spectrums of four low-energy structures show no imaginary phonon frequencies, confirming their dynamical stability [see Figs. 3(a) and (b), and Fig. S2]. Meanwhile, Table 2 lists the elastic constants of the four structures of CrTe, which satisfy the Born criterion [41, 42], indicating that they are mechanically stable. Detailed information about the Born criterion for each phase can be found in Table S2 of the supplementary material.

Two meta-stable structures including \( \text{Cmca} \) and \( \text{R3m} \) structures were predicted, which were not reported in previous works. The \( \text{Cmca} \) structure has a layered crystal lattice with each layer be held together by the vdw interaction. Its single layer consists of \( \text{Cr}_{2} \text{Te}_{4} \) cells with four edge-shared \( \text{CrTe}_{4} \) quadrangular pyramids [see Fig. 3(d)]. We have compared the energy of \( \text{Cmca} \) structure in non-magnetic (NM), FM and, different AFM states. It was founded that the FM state was unstable and would change to the NM state. The magnetic ground state of the \( \text{Cmca} \) phase is the AFM state [see Fig. 3(c)], in which the spin distribution in a single layer is opposite [see Fig. 3(d)]. The AFM state, which helps to decrease the Pauli repulsion between electrons, results in shorter Cr–Te bond lengths than that of other structures (see Table 1). Moreover, the calculated cleaved energy of a single layer is 0.464 J/m², similar to that of graphene (0.43 J/m²) [43], indicating the possible synthesis of monolayer CrTe.

On the other side, the ground state of the \( \text{R3m} \) struc-

### Table 1

The space group (SG), group number (GN), the ground magnetic state (MS), lattice parameters (LP), bonding length (\( d_{\text{CrTe}} \)) and formation enthalpies (\( \Delta H \)) of CrTe. The numbers of atoms in a conventional cell (\( N_{\text{cell}} \)) are also given.

| SG (GN) | MS     | LP       | \( d_{\text{CrTe}} \) (Å) | \( \Delta H \) (eV/atom) |
|---------|--------|----------|--------------------------|--------------------------|
| \( \text{Cmca} \) (64) | AFM    | \( a = 5.743 \) | 2.814 | –0.592 |
|          |        | \( b = 12.671 \) | 2.814 | –0.592 |
|          |        | \( c = 6.026 \) | 2.814 | –0.592 |
|          |        | \( \alpha = \beta = \gamma = 90^\circ \) | 2.814 | –0.592 |
| \( \text{P6}_3 / \text{mmc} \) (194) | FM     | \( a = b = 4.216 \) | 2.920 | –0.782 |
|          |        | \( c = 6.452 \) | 2.920 | –0.782 |
|          |        | \( \alpha = \beta = 90^\circ \) | 2.920 | –0.782 |
|          |        | \( \gamma = 120^\circ \) | 2.920 | –0.782 |
| \( \text{R3m} \) (166) | FM     | \( a = b = c = 10.184 \) | 2.925 | –0.774 |
|          |        | \( \alpha = \beta = \gamma = 23.7^\circ \) | 2.925 | –0.774 |
| \( \text{Fm} \text{3m} \) (225) | FM     | \( a = b = c = 5.817 \) | 2.909 | –0.762 |
|          |        | \( \alpha = \beta = \gamma = 90^\circ \) | 2.909 | –0.762 |

### Table 2

The independent elastic constants \( C_{ij} \) (GPa) for CrTe with various space group: cubic (\( \text{Fm} \text{3m} \)), hexagonal (\( \text{P6}_3 / \text{mmc} \)), trigonal (\( \text{R3m} \)), and orthorhombic (\( \text{Cmca} \)) phases.

| SG       | \( C_{11} \) | \( C_{22} \) | \( C_{33} \) | \( C_{44} \) | \( C_{55} \) | \( C_{66} \) | \( C_{12} \) | \( C_{13} \) | \( C_{14} \) | \( C_{23} \) |
|----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| \( \text{Cmca} \) | 53.184      | 37.381      | 61.232      | 22.160      | 34.932      | 26.810      | 16.456      | 24.746      | 13.526      |
| \( \text{P6}_3 / \text{mmc} \) | 66.858      | 81.294      | 3.891       | 23.907      | 39.082      | 41.394      | 2.920       | 41.394      | –2.418      |
| \( \text{R3m} \) | 77.804      | 77.033      | 23.907      | 39.082      | 41.394      | 2.920       | 41.394      | –2.418      | 41.394      |
| \( \text{Fm} \text{3m} \) | 119.567     | 16.885      | 21.870      | 21.870      | 21.870      | 21.870      | 21.870      | 21.870      | 21.870      |
ture is the FM state. The AFM state energy is 195.58 meV/f.u. higher than the FM state, similar to \( \text{Fm}3\text{m} \) and \( \text{P}6_3/\text{mmc} \) structure (see Fig. S3). The basic unit of \( \text{R}3\text{m} \) structure is the octahedron, similar to \( \text{Fm}3\text{m} \) and \( \text{P}6_3/\text{mmc} \) structure (see Fig. S4). As seen from Fig. 2, in both PBE and PBE+U calculations, the energy of \( \text{R}3\text{m} \) structure is slightly higher than that of \( \text{P}6_3/\text{mmc} \) (NA) structure, but lower than \( \text{Fm}3\text{m} \) (RS) structures as well as ZB structures. Thus, it was possible to synthesize the \( \text{R}3\text{m} \) structure in future experiments.

3.2 Electronic and magnetic properties

As shown in Fig. S5, the charge density difference of CrTe in various structures indicates that electrons are transferred from Cr atoms to the middle zone of Cr–Te bonds, which indicates a mixture of ionic and covalent bonding interactions between Cr and Te atoms [44]. The Cr–Te bond lengths \((d_{\text{Cr}-\text{Te}})\) of \( \text{P}6_3/\text{mmc} \), \( \text{R}3\text{m} \), and \( \text{Fm}3\text{m} \) structures is longer than that of the \( \text{Cmca} \) phase (see Table 1). The extension of \( d_{\text{Cr}-\text{Te}} \) leads to a decrease in covalent bond interaction, contrary to the ionic bonding interaction [20]. Therefore, the unpaired electrons accumulated on the Cr and Te atoms in CrTe of these three structures slightly increase compared to \( \text{Cmca} \) structure, leading to a variation of magnetism.

Figure 4 shows spin-dependent band structure and partial density of states (DOS) of CrTe in (a) \( \text{Cmca} \) and (b) \( \text{R}3\text{m} \) phases.

![Graphs showing band structure and DOS for CrTe in Cmca and R3m phases.]

**Fig. 4** The spin-dependent band structure and partial density of states (DOS) of CrTe in (a) \( \text{Cmca} \) and (b) \( \text{R}3\text{m} \) phases.

We next explored the evolution of the stable structure and phase transition of CrTe as a function of external pressure. Figure 5 plots the pressure-formation enthalpies curve of the CrTe in various structures. We set the formation enthalpies of \( \text{P}6_3/\text{mmc} \) phase to zero for a comparison.

As seen from Fig. 5, the \( \text{P}6_3/\text{mmc} \) structure was found to be the most stable phase at a range of \( 0 \sim 34 \) GPa. However, the energy differences among \( \text{P}6_3/\text{mmc} \), \( \text{R}3\text{m} \), and \( \text{Fm}3\text{m} \) structures are small. At a range of \( 30 \sim 45 \) GPa, pressure-induced phase transitions occur. The \( \text{P}6_3/\text{mmc} \) structure transforms to the \( \text{R}3\text{m} \) structure at 34 GPa and then to \( \text{Fm}3\text{m} \) structure at 42 GPa. Here the transition critical pressures were estimated by linear interpolation. During the phase transition, CrTe becomes a FM metal (see Fig. S8). We also checked the MnP-type CrTe (space group \( \text{Pnma} \)) which was also observed in the experiment [13]. We predicted that \( \text{Pnma} \) structure has higher formation enthalpy than \( \text{R}3\text{m} \) and \( \text{Fm}3\text{m} \) structures at high pressure (see Fig. 5). Thus, the high-pressure phase of CrTe should be \( \text{R}3\text{m} \) and \( \text{Fm}3\text{m} \) structures. The pressure-induced phase transition path is given below [45]:

\[
\text{P}6_3/\text{mmc} \xrightarrow{34\text{GPa}} \text{R}3\text{m} \xrightarrow{42\text{GPa}} \text{Fm}3\text{m}.
\]

**Fig. 5** The relative formation enthalpy of the CrTe in \( \text{Cmca} \), \( \text{R}3\text{m} \), \( \text{Fm}3\text{m} \) and \( \text{Pnma} \) structure with respect to that of the \( \text{P}6_3/\text{mmc} \) structure as a function of pressure.
4 Conclusion

In conclusion, we investigated the crystal structures and magnetic properties of CrTe by using particle swarm optimization algorithm combined with the first-principles calculations. It is necessary to consider the electronic correlation effect in determining the ground state of CrTe. The ground state of CrTe was founded to be the NiAs-type (space group $P6_3/mmc$) structure at ambient pressure, consistent with available experiments. Apart from that, we predicted two meta-stable phases including $Cmca$ and $R\bar{3}m$ structures. CrTe in $Cmca$ structures is a layered AFM metal. CrTe in $R\bar{3}m$ structures is a FM half-metal and may be synthesized in the future experiment, due to that its energy is slightly higher than ground-state $P6_3/mmc$ structure at ambient pressure. The CrTe in $P6_3/mmc$ structure is the most stable at low pressure. However, the ground-state structure of CrTe would transition to $R\bar{3}m$ and $Fm\bar{3}m$ structures at the pressure of about 34 and 42 GPa, respectively. Meanwhile, CrTe becomes a FM metal at high pressure.

Electronic supplementary material  See the supplemental material for the estimation of effective onsite $U_f$ value; the phonon dispersion of CrTe; the energy-volume curve of CrTe in $R\bar{3}m$ structures; the energy difference between the lowest-energy antiferromagnetic state and ground-state ferromagnetic state; the charge density difference of CrTe; the crystal orbital hamilton populations ($-COHP$) of CrTe; the band structure of CrTe in high pressure; the convex hull of Cr–Te compounds with different chemical compositions; the comparing of ground state of CrTe in previous works; the independent elastic constant and Born criterion of CrTe structure. They are available in the online version of this article at https://doi.org/10.1007/s11467-020-1088-3 and http://journal.hep.com.cn/fop/10.1007/s11467-020-1088-3 and are accessible for authorized users.

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References

1. A. Brataas, A. D. Kent, and H. Ohno, Current-induced torques in magnetic materials, Nat. Mater. 11(5), 372 (2012)
2. A. S. Núñez, R. A. Duine, P. Haney, and A. H. MacDonald, Theory of spin torques and giant magnetoresistance in antiferromagnetic metals, Phys. Rev. B 73(21), 214426 (2006)
3. B. G. Park, J. Wunderlich, X. Martí, V. Holý, Y. Kurosaki, M. Yamada, H. Yamamoto, A. Nishide, J. Hayakawa, H. Takahashi, A. B. Shick, and T. Jungwirth, A spin-valve-like magnetoresistance of an antiferromagnet-based tunnel junction, Nat. Mater. 10(5), 347 (2011)
4. E. V. Gomonay and V. M. Loktev, Spintronics of antiferromagnetic systems, Low Temp. Phys. 40(1), 17 (2014)
5. Y. Wang, C. Song, J. Zhang, and F. Pan, Spintronic materials and devices based on antiferromagnetic metals, Prog. Nat. Sci. 27(2), 208 (2017)
6. N. V. Baranov, N. V. Seleznева, and V. A. Kazantsev, Magnetism and superconductivity of transition metal chalcogenides, Phys. Met. Metallogr. 119(13), 1301 (2018)
7. W. Zhang, P. K. J. Wong, R. Chua, and A. T. S. Wee, in: Spintronic 2D Materials, Materials Today, edited by W. Liu and Y. Xu, Elsevier, 2020, pp 227–251
8. M. A. Mc Guire, Cleavable magnetic materials from van der Waals layered transition metal halides and chalcogenides, J. Appl. Phys. 128(11), 110901 (2020)
9. H. Ipser, K. L. Komarek, and K. O. Klepp, Transition metal-chalcogen systems viii: The Cr–Te phase diagram, J. Less Common Met. 92(2), 265 (1983)
10. T. Kanomata, Y. Sugawara, T. Kaneko, K. Kamishima, H. Aruga Katori, and T. Goto, Giant magnetovolume effect of CrTe, J. Alloys Compd. 297(1–2), 5 (2000)
11. M. Wang, L. Kang, J. Su, L. Zhang, H. Dai, H. Cheng, X. Han, T. Zhai, Z. Liu, and J. Han, Two-dimensional ferromagnetism in CrTe flakes down to atomically thin layers, Nanoscale 12(31), 16427 (2020)
12. M. G. Sreenivasan, J. F. Bi, K. L. Teo, and T. Liew, Systematic investigation of structural and magnetic properties in molecular beam epitaxial growth of metastable zincblende CrTe toward half-metallicity, J. Appl. Phys. 103(4), 043908 (2008)
13. T. Eto, M. Ishizuka, S. Endo, T. Kanomata, and T. Kikegawa, Pressure-induced structural phase transition in a ferromagnet CrTe, J. Alloys Compd. 315(1–2), 16 (2001)
14. M. A. Mc Guire, V. O. Garlea, S. Ke, V. R. Cooper, J. Yan, H. Cao, and B. C. Sales, Antiferromagnetism in the van der Waals layered spin-lozenge semiconductor CrTe$_3$, Phys. Rev. B 95(14), 144421 (2017)
15. Z. Charifi, D. Guedouz, H. Baaaziz, F. Soyalp, and B. Hamad, Ab-initio investigations of the structural, electronic, magnetic and mechanical properties of CrX (X = As, Sb, Se, and Te) transition metal pnictides and chalcogenides, Phys. Scr. 94(1), 015701 (2019)
16. J. Dijkstra, H. H. Weitering, C. F. Bruggen, C. Haas, and R. A. Groot, Band-structure calculations, and magnetic and transport properties of ferromagnetic chromium tellurides (CrTe, Cr$_3$Te$_4$, Cr$_2$Te$_3$), J. Phys.: Condens. Matter 1(46), 9141 (1989)
17. V. Kanchana, G. Vaitheeswaran, and M. Rajagopalan, Pressure-induced structural and magnetic phase transition in ferromagnetic CrTe, J. Magn. Magn. Mater. 250, 353 (2002)
18. W. H. Xie, Y. Q. Xu, B. G. Liu, and D. G. Pettifor, Half-metallic ferromagnetism and structural stability of zincblende phases of the transition-metal chalcogenides, Phys. Rev. Lett. 91(3), 037204 (2003)
19. T. Block and W. Tremel, Large magnetoresistance at room temperature in the off-stoichiometric chalcogenide Cr$_{0.92}$Te, J. Alloys Compd. 422(1–2), 12 (2006)
20. Y. Liu, S. K. Bose, and J. Kudrnovský, First-principles theoretical studies of half-metallic ferromagnetism in CrTe, Phys. Rev. B 82(9), 094435 (2010)
21. A. Belkadi, K. O. Obodo, Y. Zaoui, H. Moukhalwa, L. Beldi, and B. Bouhafs, First-principles studies of structural, electronic and magnetic properties of the CrS, CrSe and CrTe compounds, SPIN 08(04), 1850019 (2018)
22. H. Moukhalwa, Y. Zaoui, K. O. Obodo, A. Belkadi, L. Beldi, and B. Bouhafs, Half-metallic and half-semiconductor gaps in Cr-based chalcogenides: DFT+U calculations, J. Supercond. Nov. Magn. 32(3), 635 (2019)
23. Y. Wang, J. Lv, L. Zhu, and Y. Ma, CALYPSO: A method for crystal structure prediction, Comput. Phys. Commun. 183(10), 2063 (2012)
24. Y. Wang, J. Lv, L. Zhu, and Y. Ma, Crystal structure prediction via particle-swarm optimization, Phys. Rev. B 82(9), 094116 (2010)
25. B. Gao, P. Gao, S. Lu, J. Lv, Y. Wang, and Y. Ma, Interface structure prediction via CALYPSO method, Sci. Bull. (Beijing) 64(5), 301 (2019)
26. A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov, and S. I. Shylin, Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system, Nature 525(7567), 73 (2015)
27. F. Peng, Y. Sun, C. J. Pickard, R. J. Needs, Q. Wu, and Y. Ma, Hydrogen clathrate structures in rare earth hydrides at high pressures: Possible route to room-temperature superconductivity, Phys. Rev. Lett. 119(10), 107001 (2017)
28. Y. Nishihara, Y. Yamaguchi, M. Tokumoto, K. Takeda, and K. Fukamichi, Superconductivity and magnetism of bcc Cr–Ru alloys, Phys. Rev. B 34(5), 3446 (1986)
29. A. J. Bradley, The crystal structures of the rhombohedral forms of selenium and tellurium, Lond. Edinb. Dublin Philos. Mag. J. Sci. 48(285), 477 (2009)
30. G. Kresse and J. Furthmüller, Efficient iterative schemes for \textit{ab initio} total-energy calculations using a plane-wave basis set, Phys. Rev. B 54(16), 11169 (1996)
31. G. Kresse and D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, Phys. Rev. B 59(3), 1758 (1999)
32. P. E. Blöchl, Projector augmented-wave method, Phys. Rev. B 50(24), 17953 (1994)
33. J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77(18), 3865 (1996)
34. H. J. Monkhorst and J. D. Pack, Special points for Brillouin-zone integrations, Phys. Rev. B 13(12), 5188 (1976)
35. W. F. Pickett, S. C. Erwin, and E. C. Ethridge, Reformulation of the LDA+U method for a local-orbital basis, Phys. Rev. B 58(3), 1201 (1998)
36. M. Cococcioni and S. de Gironcoli, Linear response approach to the calculation of the effective interaction parameters in the LDA+U method, Phys. Rev. B 71(3), 035105 (2005)
37. A. Togo and I. Tanaka, First principles phonon calculations in materials science, Scr. Mater. 108, 1 (2015)
38. S. Grimme, Semiempirical GGA-type density functional constructed with a long-range dispersion correction, J. Comput. Chem. 27(15), 1787 (2006)
39. P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G. K. H. Madsen, and L. D. Marks, WIEN2k: An APW+LO program for calculating the properties of solids, J. Chem. Phys. 152(7), 074101 (2020)
40. K. Choudhary, Q. Zhang, A. C. Reid, S. Chowdhury, N. Van Nguyen, Z. Trautt, M. W. Newrock, F. Y. Congo, and F. Tavazza, Computational screening of high-performance optoelectronic materials using OptB88vdW and TB-mBJ formalisms, Sci. Data 5(1), 180082 (2018)
41. F. Mouhat and F. X. Coudert, Necessary and sufficient elastic stability conditions in various crystal systems, Phys. Rev. B 90(22), 224104 (2014)
42. Z. J. Wu, E. J. Zhao, H. P. Xiang, X. F. Hao, X. J. Liu, and J. Meng, Crystal structures and elastic properties of superhard IrN$_2$ and IrN$_3$ from first principles, Phys. Rev. B 76(5), 054115 (2007)
43. T. Björkman, A. Gulans, A. V. Krasheninnikov, and R. M. Nieminen, van der Waals bonding in layered compounds from advanced density-functional first-principles calculations, Phys. Rev. Lett. 108(23), 235502 (2012)
44. K. Nakada, H. Shimizu, and H. Yamada, Electronic structure and magnetism of CrTe with NiAs-type structure, J. Magn. Magn. Mater. 272–276, 464 (2004)
45. I. Benabdelkader, H. Bendaoud, K. O. Obodo, L. Beldi, and B. Bouhafs, An \textit{ab initio} study on the transition path of carbon dioxide at high pressure: Evidence for a new intermediate P3m2 phase, Comput. Condens. Matter 21, e00429 (2019)