ISSN 1674-1056
http://cpb.iphy.ac.cn
http://iopscience.iop.org/cpb
中国物理 B
Chinese Physics
中国物理
Chinese Physics B

Seeing Dirac electrons and heavy fermions in new boron nitride monolayers

Yu-Jiao Kang(康玉娇), Yuan-Ping Chen(陈元平), Jia-Ren Yuan(袁加仁), Xiao-Hong Yan(颜晓红), Yue-E Xie(谢月娥)

Citation: Chin. Phys. B . 2020, 29(5): 057303 . **doi:** 10.1088/1674-1056/ab7e9e
Journal homepage: http://cpb.iphy.ac.cn; http://iopscience.iop.org/cpb

What follows is a list of articles you may be interested in

General principles to high-throughput constructing two-dimensional carbon allotropes

Qing Xie(谢庆), Lei Wang(王磊), Jiangxu Li(李江旭), Ronghan Li(李荣汉), Xing-Qiu Chen(陈星秋)
Chin. Phys. B . 2020, 29(3): 037306 . **doi:** 10.1088/1674-1056/ab6c4b

Adsorptions of metal adatoms on graphene-like BC_3 and their rich electronic properties: A first-principles study

Pengfei Sui(隋鹏飞), Jiaqi Dai(戴佳琦), Yinchang Zhao(赵银昌), Zhenhong Dai(戴振宏)
Chin. Phys. B . 2018, 27(9): 097311 . **doi:** 10.1088/1674-1056/27/9/097311

Electric field manipulation of multiple nonequivalent Dirac cones in the electronic structures of hexagonal CrB_4 sheet

Jinkun Wang(王锦坤), Yajiao Ke(柯亚娇), Qingxing Xie(谢晴兴), Yanli Li(李艳丽), Jiafu Wang(王嘉赋)
Chin. Phys. B . 2018, 27(9): 097304 . **doi:** 10.1088/1674-1056/27/9/097304

Bias polarity-dependent unipolar switching behavior in NiO/$SrTiO_3$ stacked layer

Xian-Wen Sun(孙献文), Cai-Hong Jia(贾彩虹), Xian-Sheng Liu(刘献省), Guo-Qiang Li(李国强), Wei-Feng Zhang(张伟风)
Chin. Phys. B . 2018, 27(4): 047304 . **doi:** 10.1088/1674-1056/27/4/047304

Van der Waals heterostructure of phosphorene and hexagonal boron nitride: First-principles modeling

Peng Zhang(张鹏), Jing Wang(王静), Xiang-Mei Duan(段香梅)
Chin. Phys. B . 2016, 25(3): 037302 . **doi:** 10.1088/1674-1056/25/3/037302

Seeing Dirac electrons and heavy fermions in new boron nitride monolayers*

Yu-Jiao Kang(康玉娇)[1,2], Yuan-Ping Chen(陈元平)[1,2], Jia-Ren Yuan(袁加仁)[2], Xiao-Hong Yan(颜晓红)[2], and Yue-E Xie(谢月娥)[1,2,†]

[1] *School of Physics and Optoelectronics, Xiangtan University, Xiangtan* 411105, *China*
[2] *Faculty of Science, Jiangsu University, Zhenjiang* 212013, *China*

(Received 15 February 2020; revised manuscript received 5 March 2020; accepted manuscript online 11 March 2020)

Most three-dimensional (3D) and two-dimensional (2D) boron nitride (BN) structures are wide-band-gap insulators. Here, we propose two BN monolayers having Dirac points and flat bands, respectively. One monolayer is named as 5–7 BN that consists of five- and seven-membered rings. The other is a Kagome BN made of triangular boron rings and nitrogen dimers. The two structures show not only good dynamic and thermodynamic stabilities but also novel electronic properties. The 5–7 BN has Dirac points on the Fermi level, indicating that the structure is a typical Dirac material. The Kagome BN has double flat bands just below the Fermi level, and thus there are heavy fermions in the structure. The flat-band-induced ferromagnetism is also revealed. We analyze the origination of the band structures by partial density of states and projection of orbitals. In addition, a possible route to experimentally grow the two structures on some suitable substrates such as the PbO_2 (111) surface and the CdO (111) surface is also discussed, respectively. Our research not only extends understanding on the electronic properties of BN structures, but also may expand the applications of BN materials in 2D electronic devices.

Keywords: boron nitride, Dirac fermion, flat band, ferromagnetism

PACS: 73.22.–f, 73.43.Cd, 71.15.Mb **DOI:** 10.1088/1674-1056/ab7e9e

1. Introduction

Boron and nitrogen are the two nearest neighbors of carbon in the periodic table of elements, and thus boron nitride (BN) has some similar structures with carbon.[1–3] For example, three-dimensional (3D) hexagonal BN (h-BN) is like graphite. They can be cut into single-layer h-BN and graphene, respectively, and the two-dimensional (2D) monolayers can be further rolled to one-dimensional nanotubes.[4–7] Beside the similar structures, both single-layer h-BN and graphene have high thermal conductivities, high chemical stabilities, and excellent mechanical properties.[8–12] However, the electronic properties of single-layer h-BN and graphene are completely different. It is known that graphene is a Dirac material with Dirac cones locating at the *K* point in the momentum space.[13–15] The super-fast Dirac electrons lead to graphene being a star material in electronics. On the contrary, h-BN is an insulator with a band gap larger than 4 eV, and thus in most cases h-BN is only used as an insulating substrate.[16–21] The insulating of h-BN originates from the electronegativity difference between boron and nitrogen atoms which breaks the symmetry of the honeycomb lattice.

In recent years, many 2D carbon monolayers other than graphene have been proposed, such as T-graphene,[22,23] phagraphene and tetra-penta-hepta (TPH) graphene,[24] and Kagome graphene,[25] and some of them have been synthesized successfully. Although these 2D carbon allotropes are still flat monolayers, they are made of triangular, tetragonal, and pentagonal carbon rings rather than only hexagonal rings. Moreover, these carbon monolayers show different electronic properties with graphene: T-graphene is a metal; Kagome graphene has a flat band around the Fermi level, which induces rich physical phenomena such as ferromagnetism, Wigner crystallization, superconducting, and anomalous quantum Hall effect.[26–34] These new physical properties extremely extend the applications of carbon materials.

Motivated by the fast development of studies on carbon materials, one could expect that, 2D BN materials should also have many allotropes, consequently there may be unusual physical properties hidden behind the structures. To the best of our knowledge, only a few works have studied new 2D BN materials. For example, Shahrokhi *et al*. studied the electronic and optical properties of five new BN allotropes,[35] and Li *et al*. studied the electronic properties of BN structures like graphyne including sp hybridization.[36] However, all the proposed new BN allotropes are still insulators or semiconductors. A question arises: Is it possible to find BN structures having special electronic properties?

In this work, we propose two 2D BN monolayers and study their electronic properties by first-principles calculations. One of the monolayers is made of five- and seven-membered rings, and thus is named as 5–7 BN structure. The other monolayer is named as Kagome BN because it is some-

*Project supported by the National Natural Science Foundation of China (Grant No. 11874314) and the Natural Science Foundation of Hunan Province, China (Grant No. 2018JJ2377).

†Corresponding author. E-mail: yueex@ujs.edu.cn

© 2020 Chinese Physical Society and IOP Publishing Ltd

what similar to the Kagome lattice. The two new BN structures not only show good stability but also exhibit interesting electronic properties. The 5–7 BN is a Dirac semimetal, whose conduction and valence bands cross on the Fermi level and thus form Dirac points. The Kagome BN has two flat bands just below the Fermi level. The flat bands generate heavy fermions and there is strongly correlated effect between the fermions. After one-hole doping, the Kagome BN becomes a half metal because the flat band splits to spin-up and spin-down bands. In addition, the possibility of synthesizing 5–7 BN on PbO_2 (111) substrate and Kagome BN on CdO (111) substrate is also discussed, respectively. With the development of the synthesis technologies, the two BN structures could be obtained soon. Their unusual electronic properties will expand the applications of BN materials to new fields.

2. Model and methods

Figures 1(a) and 1(b) show the two new BN monolayers, respectively. The ratios of boron and nitrogen atoms in both structures are 1 : 1, and both structures have B–N, B–B, and N–N bonds. The monolayer in Fig. 1(a) is made of five- and seven-membered rings, and thus is named as 5–7 BN. The monolayer in Fig. 1(b) consists of boron triangular rings and nitrogen dimers, and the rings are linked together by the dimers. When a nitrogen dimer and two boron atoms at the two ends of the dimer are contracted to one lattice, the structure becomes a standard Kagome lattice.[37,38] Therefore, the structure in Fig. 1(b) is named as Kagome BN.

Our calculations were performed within the density-functional theory (DFT) as implemented with the Perdew–Burke–Ernzerhof (PBE) approximation to the exchange–correlation functional.[39,40] The core-valence interactions were described by the projector augmented wave (PAW) potentials as carried under the Vienna *ab initio* simulation package (VASP) code.[41] Plane waves with a kinetic energy cutoff of 600 eV were used as the basis set. For the Brillouin zone integration, 5–7 BN and Kagome BN were done with $11\times11\times1$ and $5\times5\times1$ Γ-centered Monkhorst–Pack k-point meshes, respectively.[42] The atomic positions were fully optimized by the conjugate gradient method,[43] and the energy and force convergence criteria were set to be 10^{-6} eV and 10^{-3} eV/Å, respectively. Periodic boundary conditions (PBC) were used and empty space of 20 Å was introduced in the direction perpendicular to the monolayers, which ensures that the interaction between the periodic images of the sheet is negligible. To investigate the thermal stability, we carried out *ab initio* molecular dynamics (AIMD) simulations based on a canonical ensemble,[44] a 3×3 supercell containing 72 atoms was used for 5–7 BN and a 2×2 supercell containing 48 atoms was used for Kagome BN, and the AIMD simulations were performed with a Nose–Hoover thermostat from 300 K to 1800 K.

3. Results and discussion

After being fully optimized, the two BN monolayers in Fig. 1 are still planar structures. The space groups of 5–7 BN in Fig. 1(a) and Kagome BN in Fig. 1(b) are *Cmmm* (D2H-19) and $P6/mmm$ (D6H-1), respectively. The primitive cells of the two structures are shown in the dashed-line boxes. The lattice constants of 5–7 BN are $a_1 = b_1 = 4.90$ Å, while those of Kagome BN are $a_2 = b_2 = 9.97$ Å. In the 5–7 BN, there are two types of B–N bonds whose bond lengths are 1.42 Å and 1.50 Å, respectively. The two bonds can be comparable with the B–N bond in h-BN sheet whose bond length is 1.45 Å. In the Kagome BN, there is only one type of B–N bond whose bond length is 1.33 Å. The shorter B–N is similar to the acetylene bond in graphyne.[45] The calculated cohesive energies of 5–7 BN and Kagome BN are 7.55 eV and 6.90 eV, respectively. These cohesive energies are lower than that of the h-BN monolayer (7.90 eV), which means that the two new monolayer structures are metastable.

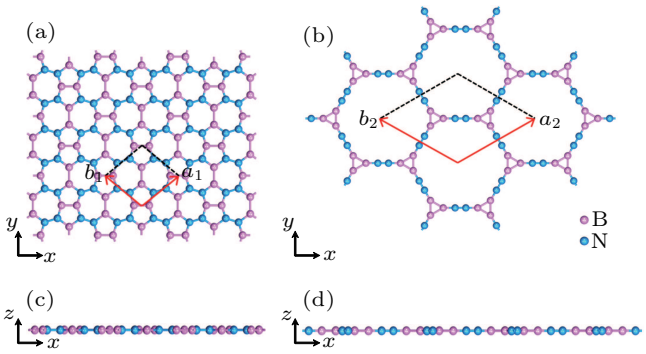


Fig. 1. (a) Top view and (c) side view of 5–7 BN, blue is for N and pink is for B atoms. Its primitive cell is shown by the dashed lines in (a). (b) Top view and (d) side view of Kagome BN. Its primitive cell is shown by the dashed lines in (b).

To confirm the structural stabilities of the two BN structures, their dynamic stabilities are examined by phonon spectrum calculations. One can find that, in Figs. 2(a) and 2(b), the phonon dispersions of both structures have no soft mode, which indicates that they are dynamic stable. The thermal stabilities of the two structures are also examined by utilizing AIMD simulation in a canonical ensemble. For the 5–7 BN structure, we do not observe any structural decomposition after heating up to the targeted temperature of 1500 K for 20 ps (see Fig. S1(a)). The structure reconstruction only occurs at 1700 K during the 20 ps simulation, as shown in Fig. S1(b). For the Kagome BN structure, we do not observe any structural decomposition when heated up to 1200 K, but reconstruction occurs at 1300 K (see Figs. S1(c) and S1(d)). Therefore, the 5–7 BN and Kagome BN have rather high thermodynamic stability and outstanding dynamic and thermal stabilities.

The band structure of the 5–7 BN is calculated, and the result is shown in Fig. 3(a). Along the high-symmetry line Γ–X and high-symmetry point Y, the conduction and valence bands

cross at D1 and D2, and result in two Dirac points whose 3D band structures are shown in Fig. 3(d). Because of the time reversal and inversion symmetries,[46,47] there are total four Dirac points in the first Brillouin zone (BZ) (see Fig. 3(c)). The calculated velocities of the Dirac electrons are approximate 4×10^5 m/s. To the best of our knowledge, all the former proposed 2D BN structures are not Dirac materials. This is the first BN material in which Dirac electrons can be found.

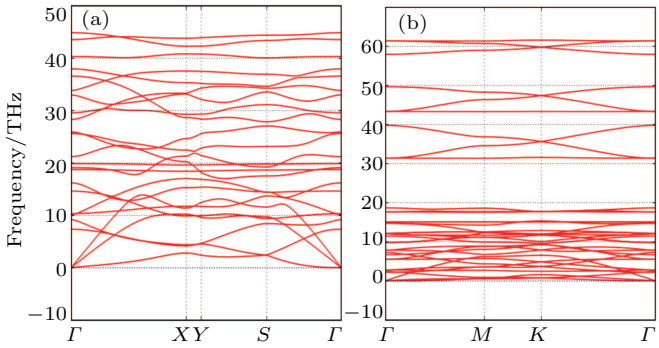


Fig. 2. Phonon dispersions of (a) 5–7 BN and (b) Kagome BN, where no soft mode is found.

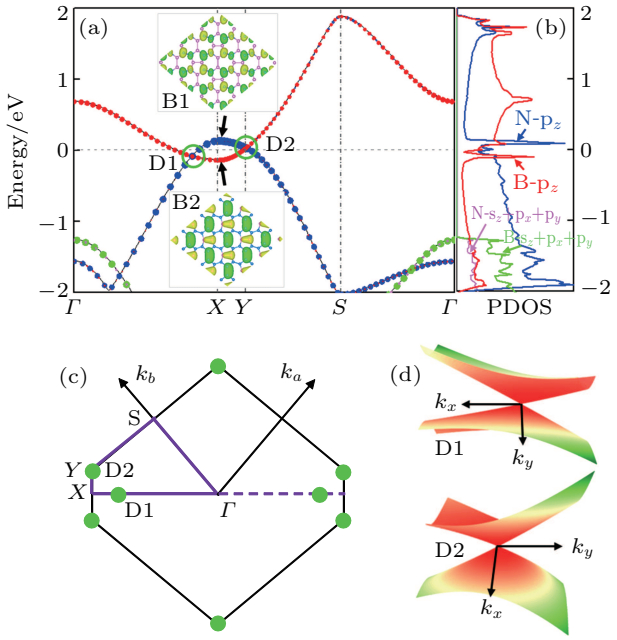


Fig. 3. (a) Projected band structure of 5–7 BN calculated by DFT, inset: the wave functions for the states from B1 and B2. (b) PDOS for B atoms and N atoms. The colors of the energy bands in (a) correspond to the colors of the projected atomic orbitals in (b). (c) Total Dirac points in the first Brillouin zone. (d) The 3D band structures for D1 and D2.

To reveal the origin of the Dirac cones in the 5–7 BN, we first calculate its partial density of states (PDOS), as shown in Fig. 3(b). One can find that the energy bands around the Fermi level are mainly contributed by the p_z orbitals of the B and N atoms. The projected energy bands in Fig. 3(a) further illustrate that the two crossing bands of the Dirac points result from different atoms: the band with red dots is mainly induced by the p_z orbital of the B atoms, while the band with blue dots is mainly induced by the p_z orbital of the N atoms. In fact, the conduction and valence bands of h-BN are contributed by the p_z orbitals of the B and N atoms, respectively (see Fig. S2). Although the B–N bond in h-BN is a covalent bond, it is more like an ionic bond in which electrons localize on the N atoms. The energy of the occupied state in N atoms is much lower than that of the unoccupied state in B atoms, and thus a wide gap appears, as shown in Fig. S2(c). In the 5–7 BN structure, there exist B–B and N–N bonds. The insets in Fig. 3(a) illustrate that a bonding state is formed in the B–B bonds while an anti-bonding state is formed in the N–N bonds. This results in the energy of the B atoms decreasing while that of the N atoms increasing (see Fig. 3(a)). In this case, band crossing occurs and Dirac points form.[48,49]

The band structure of the Kagome BN is shown in Fig. 4(a). One can find that there are two flat bands just below the Fermi level. Some other bands cross at K point, but the crossing points are far from the Fermi level. Figures 4(b) and 4(c) present PDOS of Kagome BN. It illustrates that, the top flat band is attributed by the $p_{x/y}$ orbitals of the B and N atoms, while the bottom flat band is attributed by the p_z orbitals of the B and N atoms.

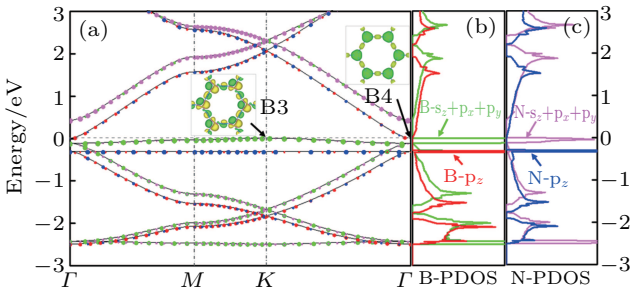


Fig. 4. (a) Projected band structure of Kagome BN calculated by DFT. PDOS for B atoms (b) and N atoms (c), respectively. The colors of the energy bands in (a) correspond to the colors of the projected atomic orbitals in (b) and (c). Inset: the wave functions for the states from B3 and B4 in (a).

In a flat band, the electron velocities are approximately equal to zero, i.e., the electrons are heavy fermions that are inverse to Dirac fermions.[50] The flat band will give rise to a series of many-body phenomena, such as ferromagnetism,[51] superconducting,[52] Wigner crystallization,[53] and anomalous quantum Hall effect.[54] In general, spin polarization of common bands is typically not favored because the kinetic energy cost is often larger than the exchange energy gain.[55] However, the flat-band physics gives another picture: when electrons fill in the flat band, the kinetic energy penalty of spin polarization does not exist anymore, hence the exchange interaction stabilizes the polarized state. In Fig. 5, we calculate the band structure of the Kagome BN when a hole is doped in the structure. One can find that the spin-up and spin-down energy bands split. The splitting of the top flat band is the largest (~ 0.6 eV). The Kagome BN becomes ferromagnetic. The magnetic moments of the atoms are calculated, and the

results indicate that magnetic moments of the B and N atoms are $0.68\mu_B$ and $-0.04\mu_B$, respectively. The B atoms possess strong magnetism.

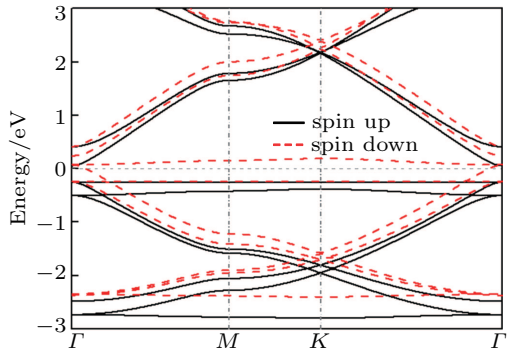


Fig. 5. Band structure of Kagome BN after one-hole doping, where the solid and dashed lines represent spin-up and spin-down energy bands, respectively. The flat band has the biggest spin splitting at about 0.57 eV.

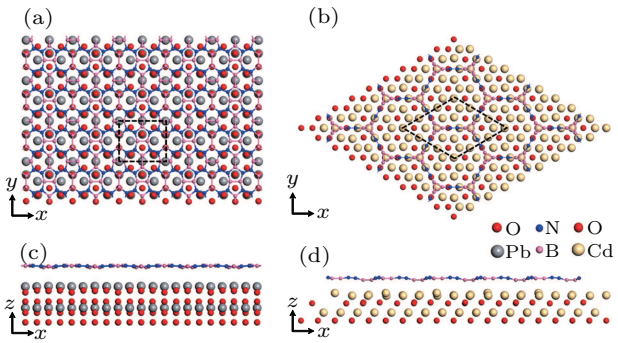


Fig. 6. (a) Top view and (c) side view of 5–7 BN on the PbO_2 (111) substrate. Its primitive cell is shown by the dashed line in (a). (b) Top view and (d) side view of Kagome BN on the CdO (111) substrate. Its primitive cell is shown by the dashed line in (b).

The above discussions on the stabilities of the two new BN structures have demonstrated the feasibility to synthesize the structures. Considering that many 2D monolayers have been synthesized on substrates,[56,57] we also investigate the possibilities to grow the two new monolayers on some suitable substrates. It is found that the lattice parameters of a $2\times\sqrt{3}$ supercell of a PbO_2 (111) substrate ($a_1' = 7.35$ Å, $b_1' = 6.36$ Å) are very close to those of 5–7 BN structure's conventional cell ($a_1 = 7.56$ Å, $b_1 = 6.23$ Å). The mismatches between them are -2.77% and 2.08% in x and y orientations, respectively (the negative percentage means the lattice constant of the substrate is shorter than the corresponding lattice parameter of 5–7 BN structure). A 5–7 BN placing on the PbO_2 (111) substrate is shown in Figs. 6(a) and 6(c). The adhesion energy between the 5–7 BN and substrate is -0.98 eV/atom. Similarly, the lattice parameters of a 3×3 supercell of a CdO (111) substrate ($a_2' = b_2' = 3.34$ Å) are very close to those of the primitive cell of the Kagome BN. The mismatch between them is smaller than 0.5%. A Kagome BN placing on the CdO (111) substrate is shown in Figs. 6(b) and 6(d). The adhesion energy between the Kagome BN and substrate is -0.42 eV/atom. These calculated energies can be comparable with those of other monolayers on oxide substrates (-0.8 eV/atom and -0.26 eV/atom) in Refs. [58,59], and thus we believe that the two predicted BN structures can be synthesized successfully.

4. Conclusion

In summary, we propose two 2D BN structures by using first-principles calculations. One is 5–7 BN made of five- and seven-membered rings, and the other is Kagome BN whose lattice is like the Kagome lattice. Both structures show good dynamical and thermal stabilities. More interestingly, the two structures reveal unusual electronic properties different from those in the former 2D BN allotropes. Most former BN allotropes are insulators or semiconductors. The 5–7 BN structure is a Dirac material, whose electron velocities are approximate 10^5 m/s. The band crossing is originated from the bonding states in the B–B bonds and antibonding states in the N–N bonds. The Kagome BN structure is a flat-band system in which two flat bands exist just below the Fermi level. There are heavy fermions with very low velocities in the structure. After one-hole doping, the top flat band splits to spin-up and spin-down flat bands, and thus ferromagnetism occurs. Dirac fermions and flat-band-induced ferromagnetism in BN allotropes have never been reported in the previous literatures. We also propose a promising approach to prepare the two new monolayers by epitaxial growth on a PbO_2 (111) substrate and a CdO (111) substrate, respectively. Our work extends people's understanding on the BN structures, and will also extend the applications of BN allotropes in different fields.

References

[1] Pakdel A, Zhi C, Bando Y and Golberg D 2012 *Mater. Today* **15** 256
[2] Xie C, Ma M, Liu C, Pan Y, Xiong M, He J, Gao G, Yu D, Xu B, Tian Y and Zhao Z 2017 *J. Mater. Chem. C* **5** 5897
[3] Dai J, Wu X, Yang J and Zeng X C 2013 *J. Phys. Chem. Lett.* **4** 3484
[4] Rubio A, Corkill J L and Cohen M L 1994 *Phys. Rev. B* **49** 5081
[5] Han W, Bando Y, Kurashima K and Sato T 1998 *Appl. Phys. Lett.* **73** 3085
[6] Meyer J C, Chuvilin A, Algara-Siller G, Biskupek J and Kaiser U 2009 *Nano. Lett.* **9** 2683
[7] Alem N, Erni R, Kisielowski C, Rossell M D, Gannett W and Zettl A 2009 *Phys. Rev. B* **80** 155425
[8] Allen M J, Tung V C and Kaner R B 2010 *Chem. Rev.* **110** 132
[9] Zhu Y, Murali S, Cai W, Li X, Suk J W, Potts J R and Ruoff R S 2010 *Adv. Mater.* **22** 3906
[10] Golberg D, Bando Y, Huang Y, Terao T, Mitome M, Tang C and Zhi C 2010 *ACS Nano* **4** 2979
[11] Hu M L, Yu Z, Zhang K W, Sun L Z and Zhong J X 2011 *J. Phys. Chem. C* **115** 8260
[12] Moradian R, Shahrokhi M, Sadat Charganeh S and Moradian S 2012 *Physica E* **46** 182
[13] Geim A K 2009 *Science* **324** 1530
[14] Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 *Rev. Mod. Phys.* **81** 109
[15] Das Sarma S, Adam S, Hwang E H and Rossi E 2011 *Rev. Mod. Phys.* **83** 407
[16] Zhou J, Wang Q, Sun Q and Jena P 2010 *Phys. Rev. B* **81** 085442
[17] Li X, Wu X, Zeng X C and Yang J 2012 *ACS Nano* **6** 4104
[18] Zeng H, Zhi C, Zhang Z, Wei X, Wang X, Guo W, Bando Y and Golberg D 2010 *Nano Lett.* **10** 5049

[19] Song L, Ci L L, Lu H, Sorokin P B, Jin C, Ni J, Kvashnin A G, Kvashnin D G, Lou J, Yakobson B I and Ajayan P M 2010 *Nano Lett.* **10** 3209
[20] Golberg D, Bando Y, Huang Y, Xu Z, Wei X, Bourgeois L, Wang M S, Zeng H, Lin J and Zhi C 2010 *Isr. J. Chem.* **50** 405
[21] Wan H, Zhou B, Liao W and Zhou G 2013 *J. Chem. Phys.* **138** 034705
[22] Liu Y, Wang G, Huang Q, Guo L and Chen X 2012 *Phys. Rev. Lett.* **108** 225505
[23] Gu Q, Xing D and Sun J 2019 *Chin. Phys. Lett.* **36** 097401
[24] Fan Q, Martin-Jimenez D, Ebeling D, Krug C K, Brechmann L, Kohlmeyer C, Hilt G, Hieringer W, Schirmeisen A and Gottfried J M 2019 *J. Am. Chem. Soc.* **141** 17713
[25] Chen Y, Xu S, Xie Y, Zhong C, Wu C and Zhang S B 2018 *Phys. Rev. B* **98** 035135
[26] Majidi R 2017 *Theor. Chem. Acc.* **136** 109
[27] Wu C, Bergman D, Balents L and Das Sarma S 2007 *Phys. Rev. Lett.* **99** 070401
[28] Bandyopadhyay A, Nandy A, Chakrabarti A and Jana D 2017 *Phys. Chem. Chem. Phys.* **19** 21584
[29] Zhou M, Liu Z, Ming W, Wang Z and Liu F 2014 *Phys. Rev. Lett.* **113** 236802
[30] Maruyama M, Cuong N T and Okada S 2016 *Carbon* **109** 755
[31] Tasaki H 1992 *Phys. Rev. Lett.* **69** 1608
[32] Wigner E 1934 *Phys. Rev.* **46** 1002
[33] Mielke A 1991 *J. Phys. A-Math. Gen.* **24** L73
[34] Huang S, Xie Y, Zhong C and Chen Y 2018 *J. Phys. Chem. Lett.* **9** 2751
[35] Shahrokhi M, Mortazavi B and Berdiyorov G R 2017 *Solid State Commun.* **253** 51
[36] Li X D and Cheng X L 2018 *Chem. Phys. Lett.* **694** 102
[37] Chern G W, Mellado P and Tchernyshyov O 2011 *Phys. Rev. Lett.* **106** 207202
[38] Chen Y, Sun Y Y, Wang H, West D, Xie Y, Zhong J, Meunier V, Cohen M L and Zhang S B 2014 *Phys. Rev. Lett.* **113** 085501
[39] Kresse G and Hafner J 1993 *Phys. Rev. B* **47** 558
[40] Hammer B, Hansen L B and Nørskov J K 1999 *Phys. Rev. B* **59** 7413
[41] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865
[42] Monkhorst H J and Pack J D 1976 *Phys. Rev. B* **13** 5188
[43] Dai Y H, Liao L Z and Li D 2004 *Numer. Algorithms* **35** 249
[44] Nosé S 1984 *J. Chem. Phys.* **81** 511
[45] Narita N, Nagai S, Suzuki S and Nakao K 1998 *Phys. Rev. B* **58** 11009
[46] Zyuzin A A, Wu S and Burkov A A 2012 *Phys. Rev. B* **85** 165110
[47] Turner A M, Zhang Y and Vishwanath A 2010 *Phys. Rev. B* **82** 241102
[48] Sun K, Yao H, Fradkin E and Kivelson S A 2009 *Phys. Rev. Lett.* **103** 046811
[49] Zhang H, Xie Y, Zhang Z, Zhong C, Li Y, Chen Z and Chen Y 2017 *J. Phys. Chem. Lett.* **8** 1707
[50] White S R and Sham L J 1981 *Phys. Rev. Lett.* **47** 879
[51] Nomura K and MacDonald A H 2006 *Phys. Rev. Lett.* **96** 256602
[52] Murphy D W, Sunshine S, van Dover R B, Cava R J, Batlogg B, Zahurak S M and Schneemeyer L F 1987 *Phys. Rev. Lett.* **58** 1888
[53] Filinov A V, Bonitz M and Lozovik Y E 2001 *Phys. Rev. Lett.* **86** 3851
[54] Laughlin R B 1983 *Phys. Rev. Lett.* **50** 1395
[55] Edelstein V M 1990 *Solid State Commun.* **73** 233
[56] Tao L, Cinquanta E, Chiappe D, Grazianetti C, Fanciulli M, Dubey M, Molle A and Akinwande D 2015 *Nat. Nanotechnol.* **10** 227
[57] Lu X, Utama M I B, Lin J, Gong X, Zhang J, Zhao Y, Pantelides S T, Wang J, Dong Z, Liu Z, Zhou W and Xiong Q 2014 *Nano Lett.* **14** 2419
[58] Zhukovskii Y F, Kotomin E A, Fuks D, Dorfman S, Marshall Stoneham A, Sychev O and Borstel G 2004 *Appl. Surf. Sci.* **226** 298
[59] Ouahab A, Mottet C and Goniakowski J 2005 *Phys. Rev. B* **72** 035421