Materials Research Express

PAPER

Structural and electronic properties of Stanene-BeO heterobilayer

Bipradip Chakraborty¹, Madhurjya M Borgohain¹ and Nirab C Adhikary* ²

¹ Department of Applied Sciences, Gauhati University, Guwahati, Assam, 781014, India
² Physical Sciences Division, Institute of Advanced Study in Science and Technology, Paschim Boragaon, Garchuk, Guwahati, Assam 781035, India

E-mail: nirab_iast@yahoo.co.in

Keywords: first-principle study, stanene, spin-orbit coupling, band gap

Abstract

Properties of Sn/BeO heterostructure formed with beryllium oxide (BeO) monolayer and 2D stanene (Sn) is studied in this work. The first-principle study is employed here to systematically investigate the structural stability and electrical properties of the Sn/BeO heterostructure. The results from simulations reveal that the introduction of BeO not only leads to a significant bandgap opening of 98 meV, but it also retains the various intrinsic electrical properties of stanene to a large extent. The effect of spin–orbit coupling (SOC) is studied both in pristine stanene as well as in Sn/BeO heterostructure. The Sn/BeO heterostructure shows the Rashba-type of spin-splitting under SOC, which is very promising for application in spintronic devices. Moreover, it is also observed that the bandgap can be tuned by applying external strain and electric field, while the characteristic Dirac cone is maintained throughout. The application of an external electric field is found to be more effective in bandgap modulation. It leads to a linear change in the bandgap, with a bandgap value of 402 meV for 4 V nm⁻¹. The results obtained from our study indicate that Sn/BeO heterostructure can be a suitable material for the development of spintronic devices.

1. Introduction

Researchers of late, have started paying attention to Group-IV elements based two dimensional (2D) materials such as silicene [1–7], germanene [8] and stanene [8] owing to their similarity in electronic properties with graphene and their possible application in nanoelectronic devices [9]. Among these, stanene has drawn keen interest due to its possible application as quantum hall insulator [10], topological insulator [11] and topological superconductor [12]. One of the important properties of stanene is that it maintains the inversion and time-reversal symmetry even after the inclusion of spin-orbit coupling (SOC). However, when the inversion symmetry breaks, it shows splitting in its energy band structure.

In the last few years number of research works related to the fabrication of stanene has been reported by some researchers. In their experimental work, Zhu et al reported the synthesis of the 2D stanene structure [13]. They successfully fabricated ultrathin Sn films with 2D stanene structure on the Bi₂Te₃ substrate by using the molecular beam epitaxy. The growth of this structure was confirmed by using scanning tunneling microscopy and angle-resolved photoemission spectroscopy and the results were found to be in good agreement with the theoretical calculations. Similarly, Saxena et al synthesized a few-layered stanene in a liquid medium by using an ultrafast laser beam with materials interactions [14]. Structural characterization done by using HRTEM confirmed the hexagonal symmetry of this stanene lattice. Unlike graphene which has a planar structure because of the presence of sp2 hybridization, stanene has a buckled honeycomb structure due to the coexistence of sp2 and sp3 hybridization. This buckled structure gives rise to many novel properties such as Spin Hall Effect and bandgap modulation in the presence of an external electric field [15]. The low buckled (LB) stanene structure has a space group of P3m1 [8]. However, stanene shows a zero bandgap without SOC, and a SOC induced bandgap of around 100 meV. This zero-bandgap limits its use in high-end devices like field-effect transistor, etc [16]. To overcome this problem, researchers have been trying different heterostructures to effectively open stanene’s
bandgap, without deteriorating its intrinsic properties. In theoretical work, Garg et al. [17] reported the bandgap opening in monolayer stanene induced by B–N doping. Similarly, Chen et al. [18] also found a bandgap opening of ~77 meV for the graphene/stanene heterobilayer. Thus, for exploiting the excellent properties of stanene, it becomes imperative for researchers to find an appropriate substrate which not only achieves tunable bandgap but at the same time maintains stanene’s intrinsic properties.

BeO is a member of the alkali earth oxides group with sp3 hybridization and it crystallizes in the Wurtzite phase. A variety of BeO based nanostructured materials has been researched extensively both theoretically and experimentally by many researchers. Zheng et al. found by using the first-principles prediction that BeO with a space group of P4/nmm (129) shows the most energetic and dynamic stability, and thus may be the most experimentally achievable 2D II-VI semiconductor [19]. Sorokin et al. also theoretically predicted single-walled BeO nanotubes, which was found to be thermodynamically stable [20]. Moreover, the fabrication technique of the BeO monolayer has been developed and some initial results have been achieved by Reinelt et al. [21] It is observed that BeO is a wide bandgap semiconductor, with good magnetic and electric properties [22, 23].

Till the date, the work on stanene/BeO heterostructure has not yet been reported by any researcher in detail. Therefore in the present work, we have considered the newly predicted beryllium oxide (BeO) monolayer for making Sn/BeO heterostructure. The structural and electrical properties of a superlattice of Sn/BeO heterostructure made by stacking Stanene and BeO monolayers are studied using DFT calculation with vdW (Van der Waals) correction. The newly formed heterostructure exhibits an opened bandgap along with the preservation of intrinsic properties of pristine stanene. The effect of SOC is studied both in pristine Stanene as well as in Sn/BeO heterostructure. Moreover, biaxial strains and an external electric field is applied to this heterostructure and is found to effectively tune the bandgap. Our results show that Sn/BeO heterostructure can be effectively made to harness the interesting properties of stanene, similar to Sn/h-BN [24] and Sn/ZnO [25].

2. Computational details

Density functional theory (DFT) with a plane-wave basis set using the Ab-initio code PWSCF package of Quantum Espresso [26] is used to perform all the calculations in this work. Norm conserving Troullier Martin pseudopotentials [27] is used to account for electron-ion interactions. The generalized gradient approximation (GGA) [28] with Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional is used to treat the exchange-correlation interaction. To take into account Van der Waals (vdW) intermolecular forces of attraction, DFT-D2 [29] dispersion correction proposed by Grimme [30] is used throughout. The plane wave basis cut off is set at 40 Ry (550 eV). The convergence threshold on force is set at $10^{-6}$ Ry/a.u. The Brillouin zone is integrated with a $12 \times 12 \times 1$ Monkhorst-Pack grid for the purpose of geometrical optimization and a $15 \times 15 \times 1$ grid for other subsequent calculations. To prevent the interaction between two adjacent heterolayers, a vacuum of 20 Å along the direction perpendicular to the surface is introduced. Spin-orbit coupling (SOC) calculation is carried out to check its effect in the electronic properties of pure stanene and the heterostructure system. For the Bader charge analysis, Henkelman code [31, 32] is used.

The interface binding energy (Eb) of the heterostructures are calculated using the equation:

$$E_b = E_{\text{Sn}/\text{BeO}} - E_{\text{Sn}} - E_{\text{BeO}}$$

(1)

where $E_{\text{Sn}/\text{BeO}}$, $E_{\text{Sn}}$, and $E_{\text{BeO}}$ represents the total energy of Sn/BeO heterostructure, pristine stanene, and BeO monolayer respectively [33, 34]. The charge density difference ($\Delta \rho$) is calculated by using the formula:

$$\Delta \rho = \rho(\text{Sn/BeO}) - \rho(\text{Sn}) - \rho(\text{BeO})$$

(2)

here $\rho(\text{Sn/BeO})$ is the total charge density of Sn/BeO heterolayer. Similarly, $\rho(\text{Sn})$ and $\rho(\text{BeO})$ is for total charge density of pristine stanene and BeO monolayer respectively.

3. Results and discussion

In this work, a two-atom hexagonal unit cell is considered for the buckled honeycomb structure of stanene. The optimized lattice constant and buckling height of pristine stanene is 4.66 Å and 0.84 Å respectively, which is in good agreement with already reported theoretical [17, 18, 24, 35–37] and experimental reports [13, 14]. Bader charge analysis shows that each Sn atom contains the same number of electrons (3.99 [e]). Similarly, four Be atoms and four O atoms are considered for the BeO unit cell. The optimized lattice constant of BeO is found to be 2.89 Å which is also in good agreement with the previous result [22]. The lattice mismatch between the two monolayers is ~37%. So, a combination of 2 × 2 lateral periodicity of stanene (a = b = 9.33 Å) and 3 × 3 lateral periodicity of BeO monolayer (a = b = 8.67 Å) is used for creating the Sn/BeO heterostructure. This
heterostructure would experience a lattice mismatch of \( \sim 7\% \). Therefore, the BeO monolayer is stretched by 7\% for ensuring heterostructure supercell commensurability.

The stability and electronic properties of the heterostructure depend on the stacking patterns. Therefore, for our study 3 (three) different stacking patterns have been considered as shown in figure 1. Similar stacking patterns have also been used by Chen et al.\[38\] In the stacking Structure-1, one \( \text{Sn}_{\text{top}} \) atom, and one \( \text{Sn}_{\text{bottom}} \) atom are placed above the center of the BeO hexagonal ring, while the center of the Sn hexagonal ring lies directly above Be–O bond. Here \( \text{Sn}_{\text{top}} \) represents Sn atoms that lie in the upper planar surface of the buckled stanene structure, whereas \( \text{Sn}_{\text{bottom}} \) represents Sn atoms that lie in the lower planar surface. In stacking Structure-2, the O atom lies below the center of the stanene hexagonal ring. Again, in stacking Structure – 3, the Be atom lies below the center of the stanene hexagonal ring. Structure-2 is found to have the lowest binding energy (Eb) among these three stacking patterns, and thus it is considered for all the calculations. To find out the optimum spacing between two adjacent layers, the binding energies with respect to different interlayer distances (\( D \)) are calculated and shown in figure 2 and also in table 1.

---

**Figure 1.** Top view of different Sn-BeO Stacking configurations: (a) Structure 1, (b) Structure 2, (c) Structure 3, and (d) Side view of Structure 2. Here \( D \) is for interlayer distance, whereas ‘b’ is for buckling distance. Sn, Be and O atoms are represented by grey, green and red color respectively.
The binding energy of our heterostructure can be compared with other recently reported works on different heterostructures [39–43]. The optimum D value is found to be 3.0 Å for the Structure-2. It has to be taken care of that the value of D is greater than the sum of covalent radii of Sn and Be or O atoms [44] so that the bond between these atoms doesn’t get formed. The buckled length (‘b’) is found to be 0.86 Å for stanene in the bilayer, which is slightly more compared to pristine stanene (0.84 Å).

The Bandgaps of pristine stanene, BeO monolayer, and Sn/BeO heterostructure are shown in figures 3(a)–(d). The band structure of stanene without SOC shows zero bandgap, which results from linear energy dispersion around the high symmetry K point, where the linear π (filled state) and π* (empty state) bands touch each other at the Fermi level (EF) [45]. However, in the presence of SOC, a sizeable direct bandgap (around 70 meV) gets opened up at the K point. The bandgap of pristine stanene without and with SOC is shown separately in figures 4(a) and (b) respectively. This result is found to be in a good agreement with 2D monolayer stanene studies of Modarresi et al [46] (70 meV bandgap in the presence of SOC), Xiong et al [47] (73 meV bandgap in the presence of SOC) as well as of Khan et al [24] (69 meV bandgap with SOC).

The band structure of the BeO monolayer shows an insulator like large bandgap value of 5 eV, with both the valence band maximum (VBM) and the conduction band minimum (CBM) located at the Γ point. Figure 3(c) shows an impressive bandgap opening of 98 meV for Sn/BeO heterostructure (without SOC) located at the K point after the introduction of the BeO substrate. The opened bandgap is larger than the bandgap of Sn/h-BN heterostructure [24]. The significant opened bandgap shows the possibility of improved on-off current ratio property, which can be harnessed in Sn/BeO made logical devices [45, 48]. As is clear from figure 3(c), the heterostructure band-gap is mainly contributed by stanene around the Fermi level. The Dirac cone retention of stanene after the introduction of the BeO substrate is worth noticing. It indicates the possible use of Sn/BeO heterostructure in nanoelectronic devices. The sublattice symmetry of stanene monolayer, which shows zero bandgap without SOC, is broken with the introduction of BeO monolayer and the resulting interaction between them. A similar phenomenon of symmetry breaking and bandgap opening has been reported for heterostructures such as Germanene/BeO [38] Graphene/h-Bn [49], Stanene/h-Bn [24] and Stanene/MoS2 [50].

Since it is well established that stanene shows sizeable bandgap (of around 0.1 eV) due to the SOC effect, therefore it is very important to include SOC effect while calculating the electronic properties of Sn/BeO.
heterostructure. After the inclusion of SOC, a band splitting phenomenon is observed for our heterostructure as shown in figure 5(b), which clearly shows the difference from figure 5(a) depicted the band structure without SOC. Such type of band splitting is known as Rashba-type splitting [51]. Stanene is a well-known system which shows a bandgap of around 0.1 eV due to the SOC effect. However, the introduction of the BeO substrate leads to the breaking of the inversion symmetry in stanene, leading to the splitting of bands. The Rashba splitting finds applications in spintronic devices. Therefore Sn/BeO heterostructure can be a promising material for spintronic devices.

Figure 3. Bandgap Structure of (a) Pristine Stanene (b) BeO monolayer (c) Sn/BeO heterobilayer (d) Enlarged Bandgap.
We have plotted the total as well as the projected density of states (PDOS) of Structure-2 in figure 6 to analyze the electronic properties and to throw some light on the interlayer interactions. As it can be seen from figure 6, the predominant contribution in PDOS around the Fermi level is from stanene. PDOS for Sn, O and Be atoms along with contributions from each orbital of the respective atoms are shown in figure 6.

Figure 7(a) shows that the major contribution in PDOS of Sn is from the p orbital. It shows the dominant role of the π orbital of stanene in the conduction and valence bands. Be atoms induce peaks around 5 eV Figure 7(b), whereas peaks around −5eV is induced by O atoms figure 7(c). The PDOS diagrams confirm that the unique and intrinsic properties of stanene are well retained in the Sn/BeO heterostructure.

To get some more insights into the bandgap opening of stanene after the introduction of BeO, the charge density difference diagram is plotted in figure 8. As is evident from figure 8, there is a significant accumulation of...
charge in the interlayer region, which is due to orbital overlap. This produces an intrinsic electric field between the two layers, the direction of which is from stanene to BeO. Moreover, there is charge accumulation on the top Sn atoms and charge depletion in the bottom Sn atoms. This difference in electric potential energies between the top and bottom Sn atoms results in the bandgap opening of stanene. This phenomenon of intrinsic dipole formation in the interface of heterolayer structure is common for other heterostructures with vdW interlayer interaction [45, 52].

Since the bandgap opening is attributed to the formation of an intrinsic dipole, the localized interlayer redistribution of charge can be modulated by application of an external electric field. Moreover, Bader charge...
analysis shows a charge transfer of 0.157 $e$ from stanene to BeO monolayer, resulting in a built-in electric field. Therefore, the application of an external electric field can be a good way for bandgap modulation.

To find out the effect of applied electric field on the bandgap of this heterostructure, an electric field perpendicular to the heterostructure is applied and bandgap is calculated as shown in figure 9(a). The application of electric field slightly affects the structure of the heterostructure and the buckling height of stanene changes from 0.84 Å to 0.92 Å. Whereas the interlayer distance changes from 3.0 Å to 3.2 Å, under the applied electric field strength from 0 to 2 V nm$^{-1}$. But significant tuning of electrical properties of the heterostructure can be achieved by the application of the electric field. As can be seen from figure 9(a), the application of a positive electric field leads to a linear change in the bandgap. The bandgap is 402 meV for 4 V nm$^{-1}$. Similarly, for the negative applied electric field, the value of bandgap is almost 0 for $-1$ V nm$^{-1}$, and it increases almost linearly up to $-4$ V nm$^{-1}$. Therefore, this almost linear relationship between the external electric field and bandgap can be used to tune the bandgap for practical application.

Bader charge analysis of stanene, top layer Sn atoms and bottom layer Sn atoms as a function of the applied electric field is done to better understand the relation between the bandgap and the applied electric field. As is evident from figure 9(b), the neutrality of electric field is perturbed with the introduction of the BeO layer. The different charge accumulation of $S_{\text{top}} = 0.093 |e|$ and $S_{\text{bottom}} = 0.06 |e|$ affects the charge neutrality of stanene and induce a bandgap opening. It explains the impressive bandgap opening of the heterostructure and retention of excellent electrical properties of stanene. With the application of a positive electric field, charge transfer takes place from stanene layer to BeO monolayer. When the applied electric field is 4 V nm$^{-1}$, the charge transfer becomes equal to 0.25 $|e|$. Therefore, the positive electric field will lead to the symmetry breaking of stanene, which leads to a bandgap opening. The increase in the positive electric field eventually leads to an increase in the bandgap. When the applied field is in the negative direction, the charge transfer of electrons from the stanene layer to the BeO monolayer is decreased. With the applied field equal to $-1$ V nm$^{-1}$, the charge difference is 0.126 $|e|$, which increases to 0.1623 $|e|$ when the applied field is equal to $-4$ V nm$^{-1}$. This implies that the symmetry of stanene is destroyed, which leads to bandgap opening. Therefore, application of external field can be an effective way for bandgap modulation.

Bandgap modulation using strain is also a commonly used method. Therefore, a study on the effect of the application of in-plane strain on the electronic properties of Sn/BeO heterostructure was done. A Homogeneous strain is applied by changing the lattice parameters using the following formula

$$\varepsilon = \left(\frac{a_{\text{strained}} - a_{\text{original}}}{a_{\text{original}}}\right) \times 100$$

where $a_{\text{strained}}$ is the lattice constant of the heterostructure under strained condition and $a_{\text{original}}$ is the original lattice constant. A negative value of $\varepsilon$ represents compressive strain, while a positive value of $\varepsilon$ represents tensile strain. As shown in figure 10(a), a tensile strain was applied to the heterostructure. The change in bandgap as a function of applied strain % is plotted in figure 10(b).

As is evident from the figure, the bandgap increases almost linearly with the increase of tensile strain. It reaches a maximum value of 180 meV for an applied tensile strain percentage value of 6%. When the strain is more than 7%, there is a significant reduction in bandgap which is caused due to significant deterioration of heterostructure integrity. Similarly, a reverse trend i.e. reduction in bandgap with an increase of compressive strain is expected. Therefore, the application of in-plane strain can also be a suitable way for bandgap modulation.

Figure 6. Density of State for Structure 2 of Sn/BeO heterobilayer structure with contribution from Sn, Be and O separately.
Figure 7. Projected Density of State for Structure 2 with different orbital contributions from (a) Sn, (b) Be, and (c) O atom.
Figure 8. Electron Charge Density Difference ($\Delta \rho$) of Stanene/BeO (Structure 2). Blue corresponds to charge accumulation. Violet corresponds to charge depletion: (a) Top view (b) Side View.

Figure 9. (a) Bandgap versus Applied Electric Field and (b) Bader charge of the top Sn, bottom Sn, and stanene as a function of applied electric field, for Sn/BeO heterostructure.
4. Conclusions

In this work, a first-principle study is performed to systematically investigate the structural stability and electrical properties of Sn/BeO heterostructure. A significant direct bandgap opening of 98 meV along with retention of Dirac cone is obtained with the introduction of BeO monolayer which happened because of the destruction of symmetry of the two sublattices in stanene induced by weak interaction between stanene and BeO layers. Furthermore, it is found that the introduction of BeO not only leads to a significant bandgap opening, but it also retains the various intrinsic electrical properties of stanene to a large extent. The bandgap of Sn/BeO can further be modulated by the application of an external electric field and in-field strain. Effect of SOC on the electronic properties of stanene and Sn/BeO heterostructure is also investigated and the inclusion of SOC opens a bandgap of around 70 meV in case of stanene. Whereas in the case of Sn/BeO heterostructure, the inclusion of SOC leads to the Rashba-type spin splitting effect. Since the fabrication of stanene and BeO monolayer has achieved some initial positive results, we are hopeful of fabrication and use of Sn/BeO heterostructure in novel nanoelectronic devices in the near future.

Acknowledgments

The authors would like to extend their sincere gratitude to the Physical Sciences Division, Institute of Advanced Study in Science and Technology (IASST) and Department of Applied Sciences, Gauhati University for providing the computation facility for the simulation and support. One of the authors (B Chakraborty) would also like to acknowledge the MHRD, Govt. of India, for offering Research Assistantship under TEQIP-III Project.

ORCID iDs

Nirab C Adhikary @ https://orcid.org/0000-0001-6022-3474
References

[1] Kara A, Enriquez H, Seitsonen A P, Lew Yan Voon L C, Vizzini S, Aufray B and Oughaddou H 2012 Surf. Sci. Rep. 67 1
[2] Wang S K, Wang J and Chan K S 2014 New J. Phys. 16 045015
[3] Sun M L, Ren Q Q, Wang S K, Yu J and Tang W C 2016 J. Phys. D 49 445305
[4] Tang W C, Sun M L, Ren Q Q, Zhang Y J, Wang S K and Yu J 2016 RSC Adv. 6 95846
[5] Wang S, Ren C, Li Y, Tian H, Lu W and Sun M 2018 Appl. Phys. Express 11 053004
[6] Ren C et al 2018 Appl. Phys. Express 11 063006
[7] Wang S et al 2019 J Supercond. Nov Magn. 32 2947
[8] Lyu I K, Zhang S F, Zhang C W and Wang P J 2019 Annalen der Physik 1900017
[9] Ferrari A C et al 2015 Nanoscale 7 4598
[10] Ezawa M 2015 J. Supercond. Nov. Magn. 28 1249–53
[11] Rachel S and Ezawa M 2014 Phys. Rev. B 89 195303
[12] Li S, de la Cruz C, Huang Q, Chen G F, Xia T L, Luo N L and Dai P 2009 Phys. Rev. B 80 020504
[13] Zhu F, Chen W, Xu Y, Gao C, Guan D, Liu C, Qian D, Zhang S and Jia J 2015 Nat. Mater. 14 1020
[14] Saxena S, Choudhary R P and Shukla S 2016 Sci. Rep. 6 31073
[15] Nigam S, Gupta S K, Majumder C and Pandey R 2015 Phys. Chem. Chem. Phys. 17 11324
[16] Wang J, Xu Y and Zhang S 2014 Phys. Rev. B 90 035403
[17] Garg P, Choudhuri I, Mahata A and Pathak B 2017 Phys. Chem. Chem. Phys. 19 3660
[18] Chen X, Meng R, Jiang J, Liang Q, Yang Q, Tan C, Sun X, Zhang S and Ren T 2016 Phys. Chem. Chem. Phys. 18 16302
[19] Zheng H, Li X B, Chen N K, Xie S Y, Tian W Q, Chen Y, Xia H, Zhang S B and Sun H B 2015 Phys. Rev. B 92 115307
[20] Sorokin P B, Fedorov A S and Chernozatonskii L A 2006 Physics of the Solid State 48 396
[21] Reineit M, Allouche A, Oberkofler M and Linsmeier C 2009 New J. Phys. 11 043023
[22] Baijia J, Erba A, Rérat M, Orlando R and Dovesi R 2013 J. Phys. Chem. C 117 12864
[23] Wu W, Lu P, Zhang Z and Guo W 2011 ACS Appl. Mater. Interfaces 3 4787
[24] Khan A I, Chakraborty T, Acharjee N and Subrina S 2017 Sci. Rep. 7 16347
[25] Cao H, Zhou Z, Zhou X and Cao J 2017 Comput. Mat. Sci. 139 179
[26] Giannozzi P et al 2009 J. Phys.: Condens. Matter 21 395502
[27] Troullier N and Martins J L 1991 Phys. Rev. B 43 8861
[28] Perdew J P, Burke K and Ernzerhof M 1997 Phys. Rev. Lett. 77 3865
[29] Lee K, Murray E D, Kong L, Lundqvist B I and Langreth D C 2010 Phys. Rev. B 82 081101
[30] Grimme S 2006 J. Comput. Chem. 27 1787
[31] Tang W, Sanville E and Henkelman G J 2009 J. Phys.: Condens. Matter 21 084204
[32] Mahata A, Rawat K S, Choudhuri I and Pathak B 2016 J. Mater. Chem. A 4 12756
[33] Xia C, Xue B, Wang T, Peng Y and Jia Y 2015 Appl. Phys. Lett. 107 193107
[34] Chen X, Yang Q, Meng R, Jiang J, Liang Q, Tan C and Sun X 2016 J. Mater. Chem. C 4 5434
[35] Borek van den B, Houssa M, Scalise E, Pournou C, Assali I V C and Justo J F 2014 J. Phys. Chem. B 118 7439
[36] Garcia J C, Lima D B, de Assali L V C and Justo J F 2011 Phys. Rev. Lett. 101 116804
[37] Chen X, Sun X, Jiang L, Liang Q, Yang Q and Meng R 2016 J. Phys. Chem. C 120 20350
[38] Wang S et al 2019 Sci Rep 9 5208
[39] Qi et al 2019 Phys. Chem. Chem. Phys. 21 1791
[40] Ren K, Wang S, Luo Y, Xu Y, Sun M, Yu J and Tang W 2019 RSC Adv. 9 4816–23
[41] Luo Y, Wang S, Chou J P, Yu J, Sun S and Sun M 2019 J. Phys. Chem. C 123 22742–51
[42] Ren K, Sun M, Luo Y, Wang S, Yu J and Tang W 2019 Appl. Surf. Sci. 476 70–5
[43] Pyykkö P and Atsumi M 2009 Chem.—Eur. J. 15 186
[44] Gao N, Li J and Jiang Q 2014 Phys. Chem. Chem. Phys. 16 11673
[45] Modarresi M, Kakara A, Mogulov K and Roknabadi M R 2015 Comput. Mater. Sci. 101 164
[46] Xiong W, Xu G, Peng Y, Du J, Wang T, Zhang J and Jia Y 2016 Phys. Chem. Chem. Phys. 18 6534
[47] Shih C-J, Wang Q H, Son Y, Jin Z, Blankschtein D and Strano M S 2014 ACS Nano 8 5790
[48] Giovannetti G, Khomyakov P A, Brocks G, Kelly P J and Brink van den J 2007 Phys. Rev. B 76 073103
[49] Xiong W, Xia C, Du J, Wang T, Peng Y, Wei Z and Li J 2017 Nanotechnology 28 195702
[50] Ishizaka K et al 2013 Nat. Mater. 10 921
[51] Chen X F, Zhu Y F and Jiang Q 2014 RSC Adv. 4 4146