# Electronic Supplementary Information for

# Tunable Electronic and Magnetic Properties of Graphene-like $XYBe_3$ (XY=BN, AlN, SiC, GeC) Nanosheets with Carrier Doping: A First-Principles Study

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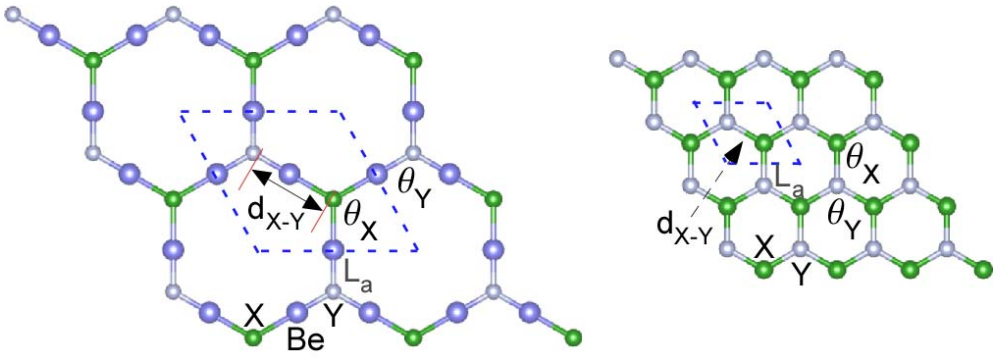
## Contents:




(a) $XYBe_3$ nanosheet (b) XY nanosheet

| | $L_a$ (Å) | $d_{X-Y}$ (Å) | $\theta_X$ (°) | $\theta_Y$ (°) | | $L_a$ (Å) | $d_{X-Y}$ (Å) | $\theta_X$ (°) | $\theta_Y$ (°) |
|---|---|---|---|---|---|---|---|---|---|
| $BNBe_3$ | 5.81 | 3.36 | 120 | 120 | BN | 2.51 | 1.45 | 120 | 120 |
| $AlNBe_3$ | 6.64 | 3.83 | 120 | 120 | AlN | 3.11 | 1.80 | 120 | 120 |
| $SiCBe_3$ | 6.51 | 3.76 | 120 | 120 | SiC | 3.09 | 1.78 | 120 | 120 |
| $GeCBe_3$ | 6.55 | 3.78 | 120 | 120 | GeC | 3.24 | 1.87 | 120 | 120 |

Table S1. The detailed structural parameters in the $XYBe_3$ and binary XY nanosheets. The corresponding mean of each parameter is marked in the above schematic diagram.

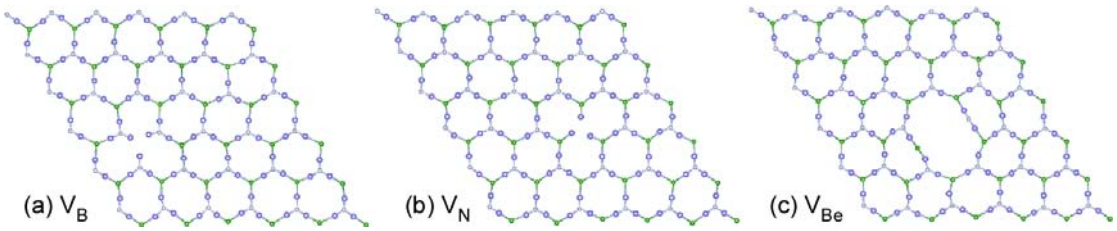



Figure S2. The final geometrical structures of $BNBe_3$ nanosheet with one single B, N, and Be vacancies. The DFTB-MD calculations on the defective $BNBe_3$ nanosheets are similar to the perfect ones in the paper. A 5×5 supercell including one B/N/Be vacancy is used in the corresponding calculations. The step time is set to 1 fs, the temperature is set to 500 K, and the whole simulated time is 10 ps. The final geometrical structures after the DFTB-MD calculations are shown above. It can be seen that although there are noticeable distortions around the vacancy, the whole structure is still kept integrated.

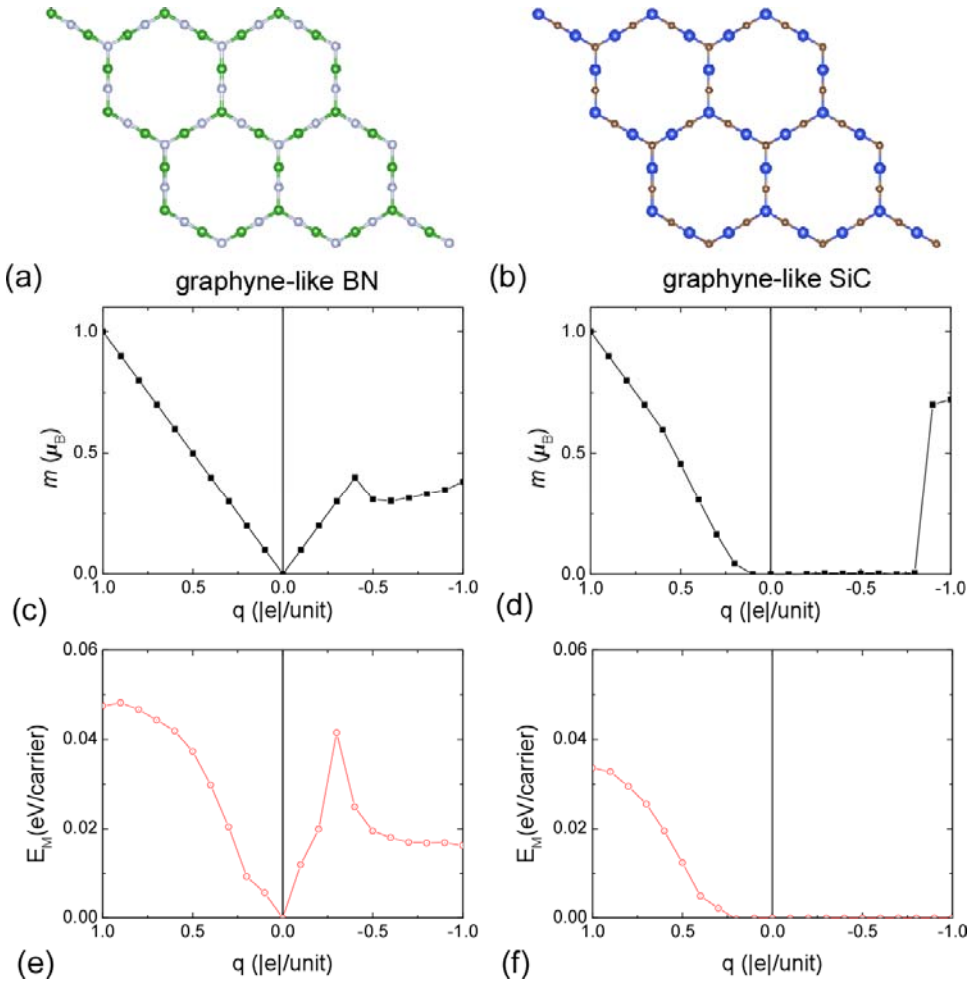



Figure S3. The geometrical structures of graphyne-like BN and SiC nanosheets are displayed in (a) and (b). The carrier-induced magnetism are depicted in (c) and (d), and the corresponding magnetic energies are shown in (e) and (f). It can be seen that for the graphyne-like BN one, both the hole and electron doping will bring the magnetism. But for the SiC case, only the hole doping can induce the valid magnetism. Comparing to the $BNBe_3$ and $SiCBe_3$ nanosheets in the paper, the carrier-induced magnetism has much weaker energetic stability in these graphyne-like BN and SiC nanosheets, whose maximum $E_M$ values are merely 0.048 and 0.034 eV/carrier under the hole doping, respectively.

| vacuum (Å) | $E_{NM}$ (eV/unit) | $E_{FM}$ (eV/unit) | $E_M$ (eV/carrier) |
|---|---|---|---|
| 15 | -21.295 | -21.340 | 0.090 |
| 17.5 | -21.077 | -21.122 | 0.090 |
| 20 | -20.873 | -20.918 | 0.090 |

Table S4. The energies of charged $BNBe_3$ nanosheets with different vacuum thicknesses. Here, we take the hole doping of 0.5 |e|/unit case as an example. The $E_{NM}$, $E_{FM}$ are the total energies of charged systems at the nonmagnetic and ferromagnetic states from the VASP calculation, and the $E_M$ is the magnetic energy per hole carrier, which is calculated as $E_M = E_{NM} - E_{FM}$. It can be seen that the vacuum thickness has significantly affected the total energy of charged systems. However, the energy difference between the NM and FM states is still a constant under the different thickness.

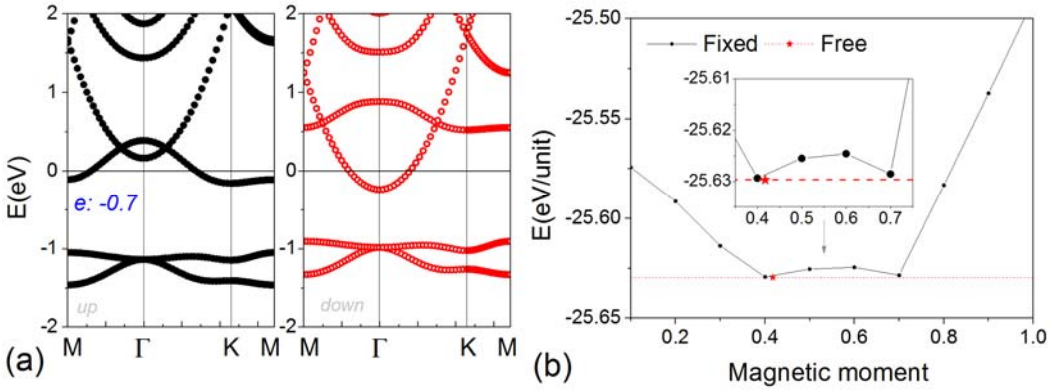



Figure S5 (a) The band structures of doped $BNBe_3$ nanosheet at the $q$ = −0.7 |e|/unit case. It can be seen that there is a nearly free electron (NFE) band appearing at the Fermi level. This NFE band is spin-polarized, which is empty in the spin up channel but partially occupied in the spin down channel. As a result, the total magnetic moment $m$ is reduced and the energy gain of magnetism $E_M$ is also decreased. The calculated total energies with the fixed magnetic moment from 0.1 to 1.0 $\mu_B$ are depicted in Fig. (b). The calculated result without any magnetic moment constraint is also marked in the picture, which is $m$ = 0.42 $\mu_B$. It can been seen that the minimum energy is just located at the $m$ = 0.42 $\mu_B$ case.