Electronic Supplementary Material (ESI) for Journal of Materials Chemistry
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Tuning the indirect-direct band gap transition of SiC, GeC and SnC monolayer in graphene-like honeycomb structure by strain engineering: a quasiparticle GW study

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Convergence tests

We have done convergence tests to 2D-SiC using LDA. Figure S1 presents total energy (Fig.S1(a)) and band gap (Fig.S1(b)) of Γ point as functions of the number of *k*-points, respectively. Similarly, we also show total energy (Fig.S1(c)) and band gap (Fig.S1(d)) of Γ point as functions of interlayer spacing, respectively. The convergence has been achieved with *k*-points sampling of 14×14×1 and interlayer spacing of 12 Å for total energy convergence tolerance (1.0×10^{-6} eV/atom). Although we finally adopt *k*-points of 24×24×1 in our LDA calculations, it is clear to see that the total energy and band gap are well converged for the number of *k*-points varied within the interval (14×14×1, 36×36×1).

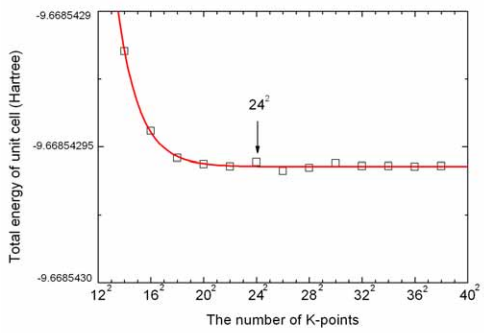

Fig. S1(a)

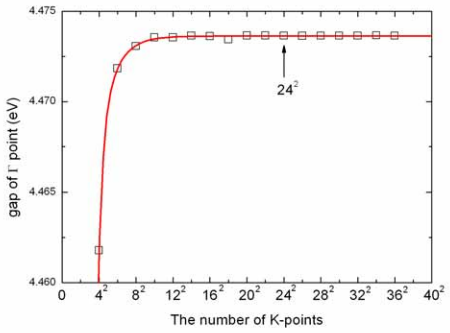

Fig.S1(b)

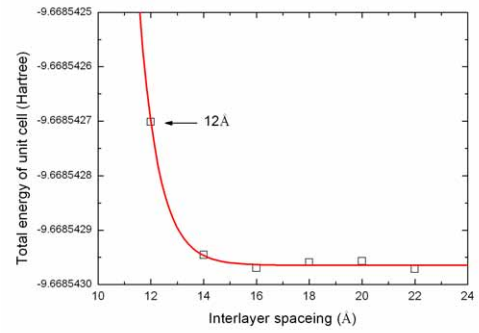

Fig. S1(c)

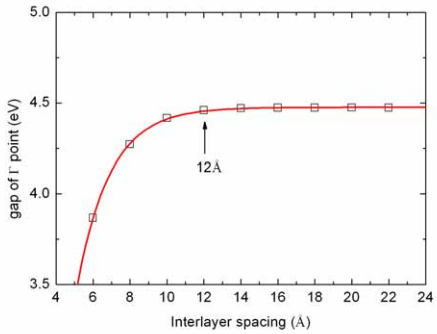

Fig.S1(d)

Fig. S1. Computational convergence tests of 2D-SiC using LDA. (a) Convergence of total energy as a function of number of k points; (b) convergence of the gap of gamma point as a function of number of k points; (c) convergence of total energy of as a function of interlayer spacing; (d) convergence of the gap of gamma point as a function of interlayer spacing. Arrows indicate the parameters finally adopted for calculations as presented in the main text.

We have done a lot of convergence tests regarding GWA calculations. In Fig.S2, we present the convergence tests of 2D-SiC in the GWA calculations. From the testing results, it is found that, convergence is achieved with 5775 plane waves (31 Hartree) to generate the independent-particle susceptibility and 2153 plane waves (16 Hartree) to generate the self-energy. We adopted 23 Hartree cut-off energy of plane waves to generate the dielectric matrix and its invervse and also to generate the exchange part of the self energy operator. The Brillouin Zone is sampled with a 24x24x1 Monkhorst-Pack k-point grid. Such sets of parameters are expected to achieve a good convergence of band gap within 0.1 eV. We have also done convergence tests for graphene, 2D-GeC and 2D-SnC, and find that pretty good convergence can be achieved if we use the same parameters as those for 2D-SiC.

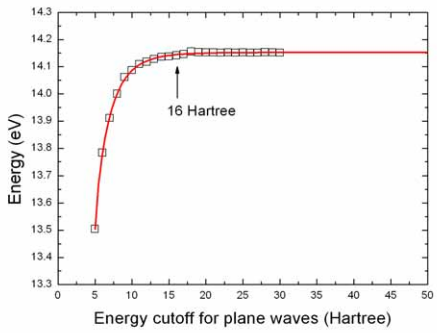

Fig.S2(a)

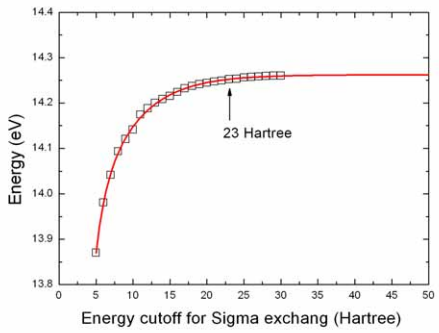

Fig.S2(b)

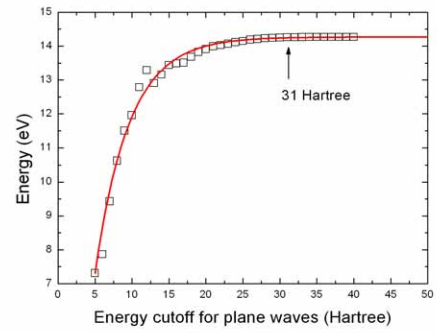

Fig.S2(c)

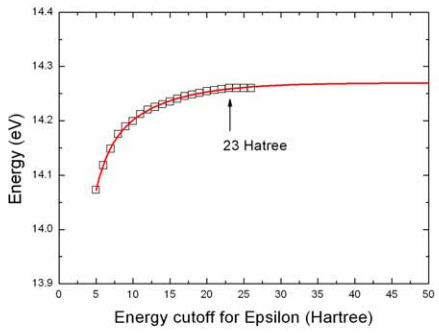

Fig.S2(d)

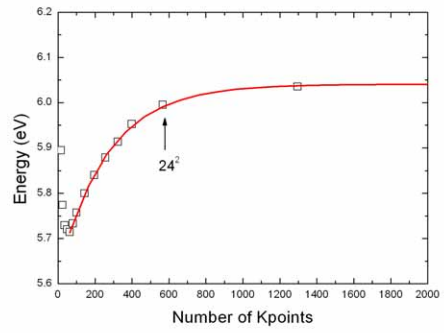

Fig.S2(e)

Fig. S2. GWA convergence of band energy as a function of various cut-off energies or k points of 2D-SiC. (a) cut-off energy of the planewave used to represent the wavefunctions that generates the self-energy; (b) cut-off energy of the planewave used to generate the exchange part of the self-energy operator; (c) cut-off energy of the planewave used to represent the wavefunctions that generates the independent-particle susceptibility; (d) cut-off energy of the planewave used to represent the independent-particle susceptibility, the dielectric matrix, and its inverse; (e) the number of k points to calculate GW correction. Arrows indicate the parameters finally adopted for this study. Such sets of parameters are expected to achieve a good convergence of band gap within 0.1 eV.