Prediction of Dirac Cones in 2D binary nanosheets

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The formation of Dirac cones in electronic band structures via isomorphous transformation is demonstrated in 2D SiC, GeC, and GeSi monolayer sheets. We combined density functional and tight-binding calculations to show that 2D SiC featuring C-C and Si-Si atom pairs possesses Dirac cones (DCs), whereas an alternative arrangement of C and Si leads to a finite band gap. The origin of Dirac points is attributed to bare interactions between Si-Si bonding states (valence bands, VBs) and C-C antibonding states (conduction bands, CBs), while the VB-CB coupling opens up band gaps elsewhere. A mechanism of atom pair coupling is proposed, and the conditions required for DC formation are discussed, enabling one to search for a class of 2D binary Dirac fermion systems solely by performing DF calculations for pure and alternative binary structures.(Xuming Qin, Yi Liu et al., J. Phys. Chem. Lett., 6, 1333-1339, 2015)