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Strain-induced Metal-Semimetal Transition of BeB₂ Monolayer

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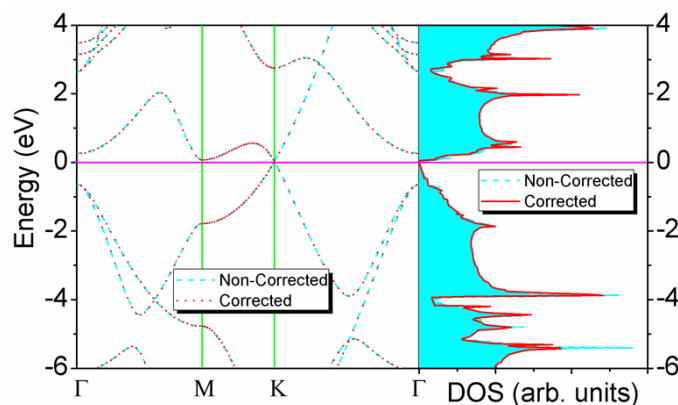


Figure S1. The band structure and total density of states (DOS) of BeB₂ monolayer under isotropic strain $\varepsilon = -5\%$ without (Non-Corrected) and with (Corrected) dipole correction. The filled-area (cyan) curve represented the DOS of BeB₂ monolayer under $\varepsilon = -5\%$ without dipole correction. The curves of band structure and DOS in two cases were basically in coincidence, which suggested that the dipole interaction between mirrors was negligible for our system due to small base plane distance and large vacuum spacing (more than 15 Å).

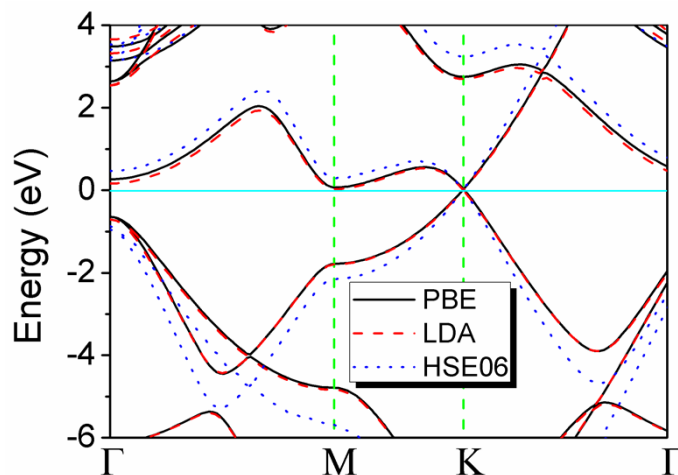


Figure S2. The band structures of BeB₂ monolayer under isotropic strain $\varepsilon = -5\%$ at PBE, LDA and HSE06 levels. The Dirac point of BeB₂ monolayer still lied at the Fermi level in the cases of LDA and Hybrid HSE06 functionals.