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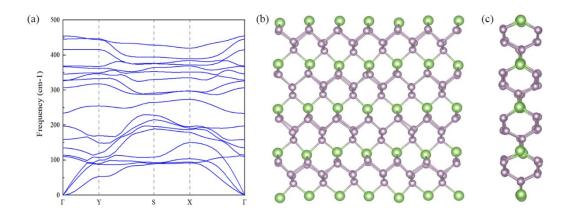


Figure S1. (a) Phonon spectra of monolayer GaP_5 . The (b) top and (c) side views of the snapshots from the AIMD simulation for monolayer GaP_5 .

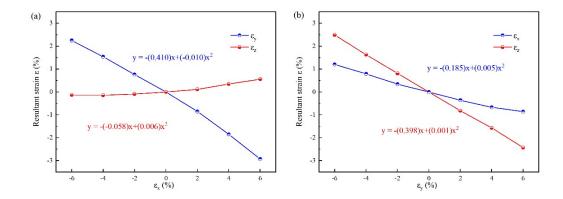


Figure S2. Mechanical response of monolayer GaP_5 under uniaxial strain along the (a) x-direction and y-direction.

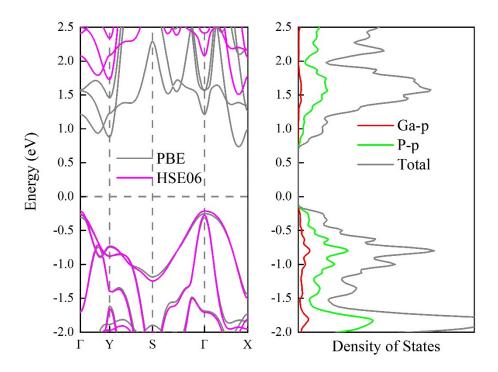


Figure 6. The band structure (PBE and HSE06) and density of states of monolayer GaP_5 .