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Strain Engineered Direct-indirect Band Gap Transition and its Mechanism in 2D Phosphorene. XIHONG PENG, QUN WEI, ANDREW COPPLE, Arizona State University — Phosphorene, a two-dimensional puckered honeycomb structure of black phosphorus, showed promising properties for applications in nano-electronics. In this work, we report strain effect on the electronic band structure of phosphorene, using first principles density-functional theory (DFT) including standard DFT and hybrid functional methods. It was found that phosphorene can withstand a tensile strain up to 30%. The band gap of phosphorene experiences a direct-indirect-direct transition when axial strain is applied. The origin of the gap transition was revealed and a general mechanism was developed to explain energy shifts with strain according to the bond nature of near-band-edge electronic orbitals. Effective masses of carriers in the armchair direction are an order of magnitude smaller than that of the zigzag axis indicating the armchair direction is favored for carrier transport. Ref: X.-H. Peng, Qun Wei, A. Copple, Phys. Rev. B 90, 085402 (2014).

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