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Few-Layer Phosphorene and Arsenene Allotropes: A Computational Study[1] DAVID TOMANEK, ZHEN ZHU, JIE GUAN, Michigan State University — There has been rising interest in layered compounds of group V elements including phosphorus and arsenic as 2D semiconductors with a substantial band gap and a high carrier mobility. Our *ab initio* density functional calculations suggest the existence of multiple sp^3 bonded phosphorene and arsenene allotropes that are stable as free-standing monolayers. We have found that α-P (black), β-P (blue), γ-P and δ-P allotropes of phosphorus are similarly stable, but display a different electronic structure. The monolayer of grey arsenic has a very similar structure as blue phosphorene and also has a wide band gap. The fundamental band gap of the compounds depends sensitively not only on the allotrope, but also the number of layers, the stacking arrangement, and in-layer strain. The energy penalty to interconnect different allotropes of the same element is unusually low, which becomes particularly valuable in assembling heterostructures with well-defined metallic and semiconducting regions in one contiguous layer.

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