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Carbon Phosphide Monolayers: Novel 2D Materials GAOXUE WANG, RAVINDRA PANDEY, Michigan Technological Univ, SHASHI P. KARNA, US Army Research Laboratory — Monolayers of carbon phosphide are investigated using the particle swarm optimization and first-principles methods. The calculated results for α-, β-, and γ- phases of carbon phosphide show novel properties including the presence of Dirac cones in the band structure. These configurations are composed of sp^2 hybridized C atoms and sp^3 hybridized P atoms in a hexagonal network with three-fold coordinated atoms. α- and β- phases are semiconducting with highly anisotropic electronic and mechanical properties whereas γ-CP is semi-metallic with a high electron mobility. Our results suggest that the group IV-V binary monolayers can be considered as a new family of 2D materials for electronics and optoelectronics applications at nanoscale.

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