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Phosphorene Oxide: Stability and electronic properties of a novel 2D material GAOXUE WANG, RAVINDRA PANDEY, Michigan Tech Univ, SHASHI P. KARNA, US Army Research Laboratory — Phosphorene, the monolayer form of the (black) phosphorus, was recently exfoliated from its bulk counterpart. Phosphorene oxide, by analogy to graphene oxide, is expected to have novel chemical and electronic properties, and may provide an alternative route to synthesis of phosphorene. In this letter, we investigate physical and chemical properties of the phosphorene oxide including its formation by the oxygen adsorption on the bare phosphorene. Analysis of the phonon dispersion curves finds stoichiometric and non-stoichiometric oxide configurations to be stable at ambient conditions, thus suggesting that the oxygen asorption may not degrade the phosphorene. The nature of the band gap of the oxides depends on the degree of the functionalization of phosphorene; indirect gap is predicted for the non-stoichiometric configurations whereas a direct gap is predicted for the stoichiometric oxide. Application of the mechanical strain and external electric field leads to tunability of the band gap of the phosphorene oxide. In contrast to the case of the bare phosphorene, dependence of the diode-like asymmetric current-voltage response on the degree of stoichiometry is predicted for the phosphorene oxide.

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