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Strain-induced topological quantum phase transition in phosphorene oxide SEOUNG-HUN KANG, JEJUNE PARK, Kyung Hee University, SUNGJONG WOO, Korea Institute for Advanced Study, YOUNG-KYUN KWON, Kyung Hee University — Using *ab initio* density functional theory, we investigate the structural stability and electronic properties of phosphorene oxides (PO_x) with different oxygen compositions x. A variety of configurations are modeled and optimized geometrically to search for the equilibrium structure for each x value. Our electronic structure calculations on the equilibrium configuration obtained for each x reveal that the band gap tends to increase with the oxygen composition of x ¡ 0.5, and then to decrease with x ¿ 0.5. We further explore the strain effect on the electronic structure of the fully oxidized phosphorene, PO, with $x = 1$. At a particular strain without spin-orbit coupling (SOC) is observed a band gap closure near the Γ point in the k space. We further find the strain in tandem with SOC induces an interesting band inversion with a reopened very small band gap (5 meV), and thus gives rise to a topological quantum phase transition from a normal insulator to a topological insulator. Such a topological phase transition is confirmed by the wave function analysis and the band topology identified by the Z_2 invariant calculation.

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