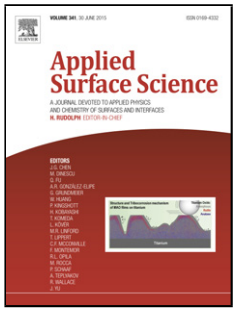

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PII: S0169-4332(16)31737-8
DOI: http://dx.doi.org/doi:10.1016/j.apsusc.2016.08.094
Reference: APSUSC 33843

To appear in: *APSUSC*

Received date: 5-6-2016
Revised date: 13-8-2016
Accepted date: 20-8-2016

Please cite this article as: Minglei Sun, Sake Wang, Jin Yu, Wencheng Tang, Hydrogenated and halogenated blue phosphorene as Dirac materials: A first principles study, Applied Surface Science http://dx.doi.org/10.1016/j.apsusc.2016.08.094

Hydrogenated and halogenated blue phosphorene as Dirac materials: A first principles study

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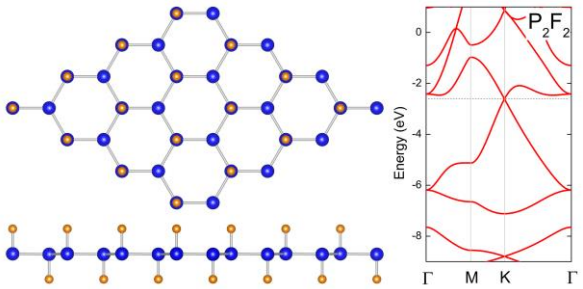
Graphical abstract



Highlights

1. The fully hydrogenated and halogenated blue phosphorenes are 2D Dirac materials.
2. The Dirac cone in fluorinated and iodinated blue phosphorenes lies exactly at the Fermi level.
3. The mass density of hydrogenated and fluorinated blue phosphorenes is rather small.

Abstract

Using first-principles calculations, we systematically investigate the structures and electronic properties of fully hydrogenated and halogenated blue phosphorene (P_2X_2). All these systems possess Dirac cone at high-symmetry *K* point with high Fermi velocity, which are mainly contributed by P *s* p_x p_y orbitals. The Dirac cone in P_2F_2 and P_2I_2 systems lies exactly at the Fermi level. Formation energy analysis denotes that all the systems are energetically stable except P_2I_2.