Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles study of atomic adsorptions on phosphorene JUN-HO LEE, YOUNG-WOO SON, Korea Inst for Advanced Study — Phosphorene with a moderate intrinsic band gap around 1eV and appropriate carrier mobility merits a next-generation electronic devices. One of the interesting characters of phosphorene is anisotropic electronic and optical properties due to its puckered atomic structures, providing an interesting realization of self-assembled low-dimensional nanostructure on it. In this study, we investigated electronic and magnetic properties of two-dimensional atomic layer formed on phosphorene by using density-functional theory calculations. We explored adsorption properties of various atoms on phosphorene and calculated energetics to predict two-dimensional atomic arrangements on top of phosphorene. In a strong spin-orbit system, we also found anisotropic spin splitting owing to its structural anisotropic.

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Date submitted: 13 Nov 2014 Electronic form version 1.4