Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electronic Structure and Rashba Spin-Orbit Coupling in Black Phosphorus ZORAN POPOVIC, JAMSHID MORADI KURDESTANY, SASHI SATPATHY, Department of Physics, University of Missouri, Columbia, MO 65221 — We investigate the electronic structure of black phosphorus using both the first-principles density-functional methods as well as a tight-binding model. The electronic structure in the gap region is described by a tight-binding Hamiltonian keeping the nearest-neighbor hopping and the p orbitals. The calculated bond-centered Wannier functions lead to the bonding picture in terms of the occupation of the p_σ bond orbitals along the phosphorous-phosphorous bonds. We find that a symmetry-breaking external electric field introduces a Rashba spin-orbit coupling; however, its magnitude is small, phosphorous being a small-Z atom. The magnitude is enhanced significantly if the phosphorous is replaced by the larger-Z bismuth.

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Date submitted: 14 Nov 2014 Electronic form version 1.4