Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Quantum Monte Carlo Studies of Bulk and Few- or Single-Layer Black Phosphorus[1] LUKE SHULENBURGER, ANDREW BACZEWSKI, Sandia National Laboratories, ZHEN ZHU, JIE GUAN, DAVID TOMANEK, Michigan State University — The electronic and optical properties of phosphorus depend strongly on the structural properties of the material. Given the limited experimental information on the structure of phosphorene, it is natural to turn to electronic structure calculations to provide this information. Unfortunately, given phosphorus' propensity to form layered structures bound by van der Waals interactions, standard density functional theory methods provide results of uncertain accuracy. Recently, it has been demonstrated that Quantum Monte Carlo (QMC) methods achieve high accuracy when applied to solids in which van der Waals forces play a significant role. In this talk, we will present QMC results from our recent calculations on black phosphorus, focusing on the structural and energetic properties of monolayers, bilayers and bulk structures.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Date submitted: 13 Nov 2014 Electronic form version 1.4