

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

***Ab-initio* Calculations of Electronic Properties of Boron Phosphide (BP)** JOHN EJEMBI, LASHAUNDA FRANKLIN, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics Southern University and A&M College, Baton Rouge, LA 70813, USA — We present results from *ab-initio*, self consistent local density approximation (LDA) calculations of electronic and related properties of zinc blende boron phosphide (BP). We employed a local density approximation (LDA) potential and implemented the linear combination of atomic orbitals (LCAO) formalism. This implementation followed the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). We discuss our preliminary results for the indirect band gap, from Γ to X, of Boron Phosphide. We also report calculated electron and hole effective masses for Boron Phosphide and total (DOS) and partial (pDOS) density of states. Acknowledgments: This research is funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE-NA0001861), LaSPACE, and LONI-SUBR.

Yuriy Malozovsky
Southern Univ & A&M Coll

Date submitted: 15 Nov 2013

Electronic form version 1.4