Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Ab-initio Calculations of Electronic Properties of InP and GaP[1]

YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, Department of Physics Southern University and A&M College, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Department of Physics Southern University and A&M College —

We present results from *ab-initio*, self consistent local density approximation (LDA) calculations of electronic and related properties of zinc blende indium and gallium phosphides (InP & GaP) 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). This method searches for the optimal basis set that yields the minima of the occupied energies. This search entails methodically increasing the size of the basis set, up to the optimal one, and the accompanying enrichment of angular symmetry and of radial orbitals. Our calculated, direct band gap of 1.398 eV (1.40 eV) for InP, at the Γ point, is in excellent agreement with experimental values. We discuss our preliminary results for the indirect band gap, from Γ to X, of GaP. We also report calculated electron and hole effective masses for both InP and GaP and the total (DOS) and partial (pDOS) densities of states.

[1]This work was funded in part by the National Science Foundation and the Louisiana Board of Regents, through LASiGMA and LS-LAMP, [EPS-1003897, No. NSF (2010-15)-RII-SUBR, and HRD-1002541] and by the Louisiana Optical Network Initiative (LONI) at SUBR.

Yuriy Malozovsky
Department of Physics Southern University and A&M College

Date submitted: 14 Nov 2012 Electronic form version 1.4