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***Ab-initio* Calculations of Electronic Properties of AlP, GaP and InP** YURIY MALOZOVSKY, Southern Univ & A&M Coll, AZIZJON SALIEV, Department of Electrical and Computer Engineering, Binghamton University, NY 13902 USA, LASHAUNDA FRANKLIN, Department of Physics Southern University and A&M College, Baton Rouge, LA 70813 USA, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 USA, GUANG-LIN ZHAO, 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 aluminum, gallium and indium phosphides (AlP, GaP & InP). 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). Our calculated, indirect band gap of 2.56 eV for AlP, and of 2.14 eV for GaP, from Γ to X, are in excellent agreement with experimental values. Our calculated direct band gap of 1.40 eV, at Γ -point for InP is also in excellent agreement with experimental value. We also report calculated electron and hole effective masses for AlP, GaP and InP and total (DOS) and partial (pDOS) densities of states. 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.

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