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Comparisons of Accurate Electronic, Transport, and Bulk Properties of XP (X=B, Al, Ga, In). YURIY MALOZOVSKY, JOHN EJEMBI, Department of Physics Southern, University and AM College, Baton Rouge, LA 70813, USA, AZIZJON SALIEV, Department of Electrical and Computer Engineering, Binghamton University, NY 13902, USA, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Department of Physics Southern, University and AM College, Baton Rouge, LA 70813, USA — We present comparisons of results from *ab-initio*, self-consistent local density approximation (LDA) calculations of accurate, electronic and related properties of zinc blende XP (X=B, Al, Ga, In) phosphides. We implemented the linear combination of atomic orbitals following the Bagayoko, Zhao, and Williams (BZW) method as enhanced by Ekuma and Franklin (BZW-EF). Consequently, our results have the full physical content of DFT and agree very well with corresponding experimental ones [AIP Advances, 4, 127104 (2014)]. Our calculated, indirect band gap of 2.02 eV for BP, 2.56 eV for AlP, and of 2.29 eV for GaP, from Γ to X-point, are in excellent agreement with experimental values. Our calculated direct band gap of 1.43 eV, at Γ , for InP is also in an excellent agreement with experimental value. We discuss calculated electron and hole effective masses, total (DOS) and partial (pDOS) densities of states, and the bulk modulus of these phosphides. Acknowledgments: NSF and the Louisiana Board of Regents, LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, DOE – National, Nuclear Security Administration (NNSA) (Award Nos. DE-NA0001861 and DE- NA0002630), LaSPACE, and LONI-SUBR.

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