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Electronic properties of InP in terms of an ab-initio LDA YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, Department of Physics, Southern University and A&M College, Baton Rouge, LA 70813, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Department of Physics, Southern University and A&M College, Baton Rouge, LA 70813 — We present results from ab-initio local density approximation (LDA) calculations of electronic and related properties of zinc blende indium phosphide (InP). Our computations employed the Ceperley and Alder LDA potential and the linear combination of atomic orbital (LCAO) formalism. The implementation of the LCAO formalism followed the Bagayoko, Zhao, and Williams (BZW) method. Consequently, we solved self consistently both the Kohn sham equation and the one giving the ground state charge density in terms of the wave functions of the occupied states. Self-consistency, for the latter equation, requires a search for the optimal basis set. This search entails increases of the size of the basis set and the related modifications of angular symmetry and of available radial functions. Our calculated, direct band gap of 1.398 eV (1.40 eV), at the ? point, is in excellent agreement with experimental values. The calculated density of states (DOS) also agree with experimental finding. The calculated electron and hole effective masses differ by 10% from some corresponding experimental ones. We discuss the equilibrium lattice constant and optical properties.

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