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Density Functional Band Gaps of AlAs HUA JIN, GUANGLIN ZHAO, DIOLA BAGAYOKO, Southern University and A&M College — We present results of ab-initio, self-consistent calculations of electronic properties of AlAs in the zinc-blende structure. Our non-relativistic calculations employed the generalized gradient approximation (GGA) of density functional potential and Bagayoko, Zhao and Williams (BZW) implementation of the linear combination of atomic orbitals (LCAO) formalism. Our calculated indirect band gaps at the X gand L points are 2.15 eV and 2.38 eV, respectively, in excellent agreement with experimental values. The calculated direct gap at Γ is 25% smaller than the experimental one. This discrepancy may be due to experimental difficulties in the determination of this gap and it is also possibly due to the fact that it is not the fundamental one and hence may not be described by a ground state calculation. We also present calculated total and partial density of states and the electron effective mass at the bottom of the conduction band at the Γ gpoint. This work was funded in part by the Department of the Navy, Office of Naval Research (ONR, Grant No. N00014-05-1-0009), NASA (Award Nos. NCC 2-1344 and NAG 5-10253), and by the National Science Foundation (Award No. HRD 0000272). The authors are indebted to Dr. S. Hasan for his excellent technical support with the computing facilities.

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