

Abstract Submitted  
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**Reexamination of the Ab-Initio Calculation of the Electronic Structure of ZnSe, Ge, and GaAs** G.L. ZHAO, L. FRANKLIN, D. BAGAYOKO, Department of Physics, Southern University and A & M College, Baton Rouge, LA 70813 — We reexamined some of the mathematical and physical properties of the ab-initio LCAO calculations for the electronic structure of ZnSe, Ge, and GaAs. The utilization of non-strongly minimal systems in the self-consistent ab-initio calculations could lead to a non-uniformity in approaching the solution in the Ritz-process. We have proposed that an optimum basis set may be needed so that the calculated electron density is converged and the significant scattering of the Ritz-coefficients may be avoided. We have applied the new method to the calculations of the electronic structure of ZnSe, Ge, and GaAs. Our calculated results of the electronic properties agree well with experimental data. Work was funded in part by US NASA (NASA Award No. NCC 2-1344), ONR (Grant No: N00014-04-1-0587], and NSF and the Louisiana Board of Regents (NSF Award Nos. HRD-0000272 and LEQSF(2002-2003)-ENH-TR-57).

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