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***Ab-initio* Calculations of Electronic Properties of Calcium Fluoride (CaF_2)** BIR BOHARA, LASHOUNDA FRANKLIN, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813, USA — We have performed first principle, local density approximation (LDA) calculations of electronic and related properties of cubic calcium fluorite (CaF_2). Our non-relativistic computations employed the Ceperley and Alder LDA potential and the linear combination of atomic orbitals (LCAO) formalism. The implementation of the LCAO formalism followed the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). We discuss the electronic energy bands, including the large band gap, total and partial density of states, electron and hole effective masses, and the bulk modulus. Our calculated, indirect (X-Γ) band gap is 12.98 eV; it is 1 eV above an experimental value of 11.8 eV. The calculated bulk modulus (82.89 GPA) is excellent agreement with the experimental result of 82.0 0.7. Our predicted equilibrium lattice constant is 5.42Å. Acknowledgments**:** This work 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-NA-0002630), LaSPACE, and LONI-SUBR.

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