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Ab-initio Computation of the Electronic, transport, and Bulk Properties of Calcium Oxide.[1] AUGUSTINE MBOLLE, DIPENDRA BANJARA, YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Department of Mathematics and Physics, Southern University and A M College, Baton Rouge, LA, 70810, USA. — We report results from ab-initio, self-consistent, local Density approximation (LDA) calculations of electronic and related properties of calcium oxide (CaO) in the rock salt structure. We employed the Ceperley and Alder LDA potential and the linear combination of atomic orbitals (LCAO) formalism. Our calculations are non-relativistic. We implemented the LCAO formalism following the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). The BZW-EF method involves a methodical search for the optimal basis set that yields the absolute minima of the occupied energies, as required by density functional theory (DFT). Our calculated, indirect band gap of 6.91eV, from towards the L point, is in excellent agreement with experimental value of 6.93-7.7eV, at room temperature (RT). We have also calculated the total (DOS) and partial (pDOS) densities of states as well as the bulk modulus. Our calculated bulk modulus is in excellent agreement with experiment.

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