THE STRUCTURAL, ELECTRONIC, AND OPTICAL PROPERTIES OF ANORTHITE $CaAl_2Si_2O_8$

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This study aims to investigate the structural, electronic, and optical properties of Anorthite $CaAl_2Si_2O_8$.
The structural and electronic characteristics are examined using density functional theory (DFT), while empirical methods, specifically the modified Moss relation, are employed for analyzing optical properties.

The exchange-correlation potential is determined through the generalized gradient approximation (PBEsol-GGA) within the density functional theory (DFT) framework, utilizing the projected augmented wave pseudopotentials (PAW) approach.

The Brillouin zone integrations were replaced by discrete summations over a special set of k-points, using the standard k-point technique of Monkhorst and Pack, where the k-point mesh used is (8 × 8 × 8). The planewave
energy cutoff to expand the wave functions is set to 120 Ry which guarantee an energy convergence threshold lower than 1.0E-4 Ry.

In this work, our calculations are carried out using DFT code: Quantum Espresso which is based on planewaves and pseudopotentials.
The calculated lattice parameters at equilibrium volume and the bulk modulus exhibit good agreement with existing literature data. Additionally, the mineral anorthite $CaAl_2Si_2O_8$ is identified as having an indirect band gap.

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