

Study on the structure, electronic and optical properties of the double perovskite Sr₂FeTeO₆ compound

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Density functional theory (DFT) calculations were performed to systematically investigate the structural, electronic, and optical properties of the double perovskite compound Sr₂FeTeO₆. Exchange–correlation effects were treated within the generalized gradient approximation using the Perdew–Burke–Ernzerhof (PBE–GGA) functional. The calculated equilibrium lattice parameters indicate a cubic structure; however, no experimental or theoretical studies reported in the literature confirm the stability of the $Fm\bar{3}m$ phase. The optical response was analyzed using several theoretical models. Furthermore, Sr₂FeTeO₆ exhibits an indirect band gap and a distinctive electronic band structure, suggesting that this compound is a promising candidate for battery-related applications.