Abstract

The focus of present PhD research work is to explore the structural, mechanical, elec-tronic, and optical properties of perovskites materials under external pressure.

A brief overview of research work is given as follows

In the first research paper, we have investigated the effects of systematic external static isotropic pressure on the phase stability, electronic band structure, and optical characteristics of BaTiO3, SrTiO3, and CaTiO3. Computational analyses were con-ducted using the Cambridge Serial Total Energy Package, employing the generalized gradient approximation and density functional theory with the Perdew-Burke-Ernzerhof exchange-correlation functional, along with ultra-soft pseudo potentials for frozen core effects. Structurally, no phase transformations were observed, with all compounds maintaining a cubic structure throughout the study. Band structure analy-sis served as a crucial tool for discerning the material nature, whether insulator, semi-conductor, or metal. Under applied pressure, the band gaps of BaTiO3, SrTiO3, and CaTiO3 experienced an increase while retaining their indirect character. Total, partial, and elemental density of states was calculated to provide a comprehensive description of the band structure.

Various optical parameters were examined to validate the authenticity of BaTiO3, SrTiO3, and CaTiO3, including real and imaginary dielectric functions, absorption, refractive index, extinction coefficient, energy loss function, and reflectivity. Discrep-ancies observed in structural parameters, band structure, and optical properties were attributed to the applied pressure, highlighting the interconnected nature of BaTiO3, SrTiO3, and CaTiO3.

In the second research paper, we have investigated the fluro-perovskite like Cesium Strontium Fluoride (CsSrF3) marks a novel endeavor, with a comprehensive investi-gation spanning structural, elastic, mechanical, anisotropic, electronic, and optical characteristics under varying stress levels from 0 to 513 GPa. This study presents a detailed analysis shedding light on the behavior of (CsSrF3) under extreme conditions, offering valuable insights into its potential applications and fundamental properties.

Structurally, CsSrF3 demonstrates remarkable stability, with no observed phase transi-tion even under significant stress. Throughout the investigation, the compound main-tains its cubic structure, showcasing its robustness and structural integrity across a wide range of pressure regimes. This inherent stability lays a strong foundation for further exploration and utilization of CsSrF3 in various technological applications. Mechanically, CsSrF3 exhibits intriguing behavior, displaying stability across most stress levels, except at 0 and 500–513 GPa. Analysis reveals that the material is nota-bly stiffer and more resistant to permanent deformation within the 0–20 GPa range before transitioning into a ductile state. This transition underscores the complex me-chanical response of CsSrF3 under varying stress conditions, providing valuable in-sights into its mechanical properties and behavior under extreme environments.

The electronic properties of CsSrF3 are characterized by its band gap, which under-goes significant alterations under external pressure. At 0 GPa, CsSrF3 possesses an indirect band gap of 5.709 eV, which progressively increases to a maximum value of 7.155 eV at 30 GPa. Further high-pressure regimes lead to the intriguing phenomenon of the band gap closing entirely, reaching a value of 0 eV. This transition from an in-sulator to a semiconductor and eventually towards a conductor highlights the pro-found impact of external pressure on the electronic structure of CsSrF3, opening ave-nues for novel electronic applications and device functionalities. The optical proper-ties of CsSrF3 under pressure are thoroughly examined, revealing significant changes in various optical parameters. The presence of its absorption edge in the UV region positions CsSrF3 as a promising candidate for UV detection applications, owing to its favorable optical characteristics and sensitivity to UV radiation. This finding under-scores the potential practical applications of CsSrF3 in the development of high-performance UV detectors, contributing to advancements in sensing technology and environmental monitoring.

In summary, the comprehensive investigation of CsSrF3 under varying pressure regimes offers valuable insights into its structural, mechanical, electronic, and optical properties. The observed stability, mechanical behavior, elec-tronic transitions, and optical characteristics under pressure highlight the multifaceted nature of CsSrF3 and its potential for diverse applications ranging from electronics to sensing. Further research in this direction holds promise for uncovering additional functionalities and optimizing the performance of CsSrF3-based devices in real-world application