Structural, Electronic, Optical and Thermodynamic Properties of SrSiO3: A DFT study

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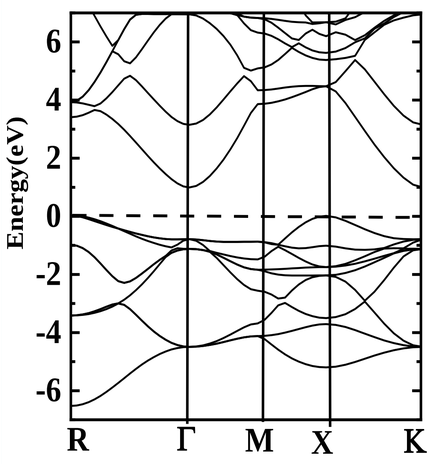
Abstract

The structural, electronic, and optical properties of cubic perovskite $SrSiO_3$ were studied using DFT with PBE exchange-correlation under GGA and mBJ. $SrSiO_3$ is thermodynamically stable with well-matched lattice parameters. It is a semiconductor with an indirect band gap, with Si–O bonds dominating the electronic structure. DOS shows oxygen's p-orbitals contribute to the valence band, and silicon's d-orbitals influence the conduction band. Optical analysis reveals strong UV absorption, high absorption coefficient, and low reflectivity, making $SrSiO_3$ a promising material for optoelectronic and UV light-harvesting applications.

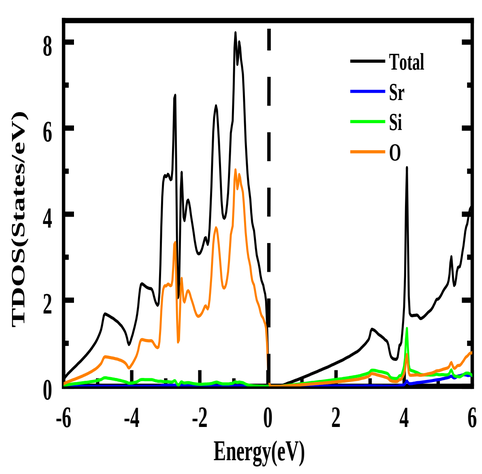
Introduction

- **Perovskite oxides (ABO_3)** with alkaline earth and rare-earth metals exhibit exceptional structural, electronic, and functional properties, making them valuable for various applications.
- **Applications** include fuel cells, sensors, spintronics, and electronic devices due to their stability, superconductivity, and magnetoresistance.
- **Computational advancements** in density functional theory (DFT) and machine learning have improved the design and understanding of these materials.
- **Experimental studies** on $SrTiO_3$, $LaMnO_3$, and $PbCrO_3$ have provided insights into their electronic and optical properties.
- **$PbGeO_3$ (germanate perovskite)** has been studied experimentally, but its cubic phase lacks detailed theoretical analysis.
- **$SrSiO_3$ perovskite** shows potential for electronic and energy applications, with DFT simulations revealing a narrow band gap and strong optoelectric response.
- **Future research** is needed to optimize perovskite oxides for advanced energy and electronic technologies through experimental and computational studies.

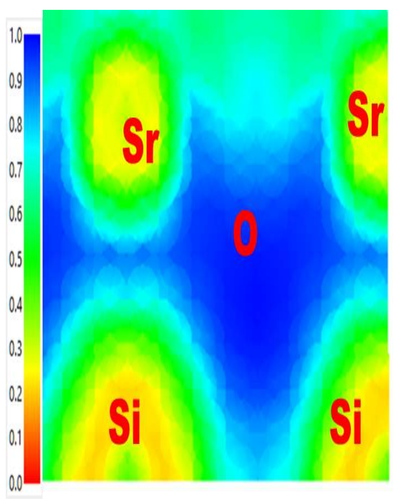
Computational information



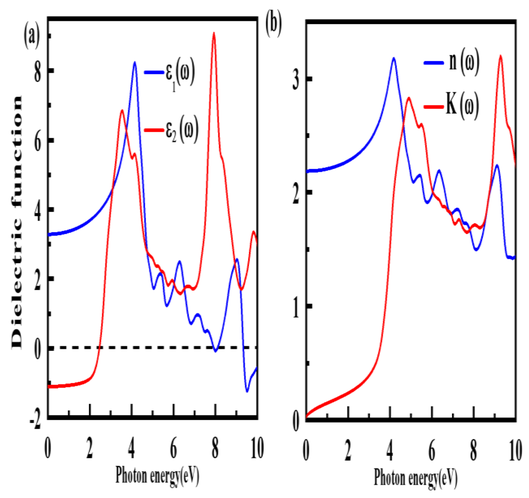
Computed band structure of $SrSiO_3$



Computed density of states for $SrSiO_3$

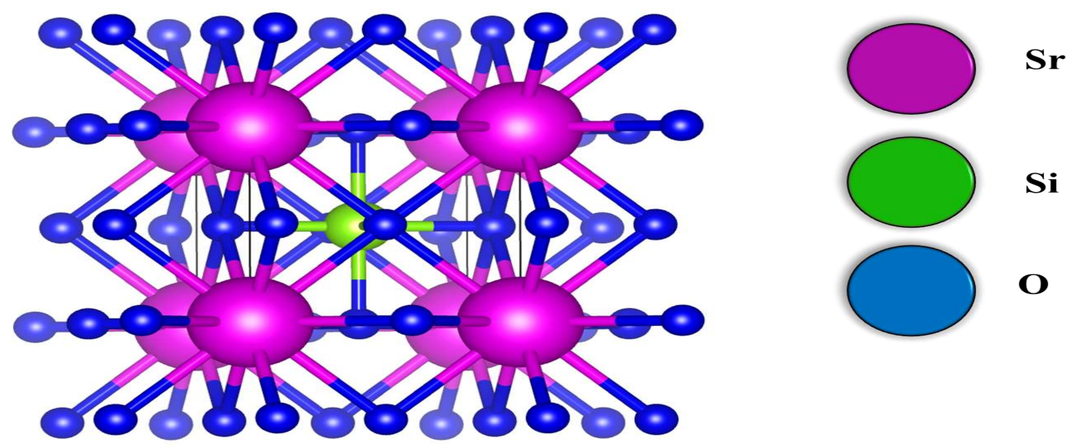


Electron density plot for SrSiO3



Computed optical properties of $SrSiO_3$

Crystal Stracture



Results

Dielectric Function (ε(ω)): The real part (ε′(ω)) reaches a maximum at **4.1 eV**, with a static dielectric constant of **3.32**. The imaginary part (ε″(ω)) has peaks at **3.2 eV** and **7.3 eV**, indicating strong UV absorption.

Refractive Index (n(ω)): The static refractive index is **2.08**, rising through the visible range and peaking at **3.2 at 6.4 eV** in the UV spectrum, making $SrSiO_3$ suitable for optical coatings.

Extinction Coefficient (k(ω)) & Absorption: k(ω) remains low in the visible spectrum but increases significantly beyond **3.2 eV**, with absorption peaks beyond **7 eV**, confirming $SrSiO_3$ as an efficient UV absorber.

Optical Band Gap: The onset of optical absorption occurs at approximately **1.28 eV**, aligning with the electronic band gap obtained using the mBJ potential.

Reflectivity (R(ω)): $SrSiO_3$ exhibits moderate reflectivity, with values increasing beyond **8 eV**, suggesting potential for high-energy optical applications.

Energy Loss Function (L(ω)): The loss function exhibits a sharp peak at **9.5 eV**, indicating strong plasmonic excitations in this range.

Potential Applications: Due to its high UV absorption, $SrSiO_3$ is a strong candidate for **UV photodetectors, anti-reflective coatings, and optoelectronic devices**.

Conclusions

We investigated the structural, electronic, and optical properties of cubic $SrSiO_3$ using DFT with GGA and mBJ approximations. $SrSiO_3$ is stable with a theoretical lattice match and an indirect band gap. DOS analysis highlights Si-O bonds shaping the valence and conduction bands. The dielectric function reveals strong UV absorption, high absorption coefficient, and low reflectivity, making it promising for optoelectronic applications. These properties suggest potential use in ultraviolet light harvesting and advanced optical devices.

References

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