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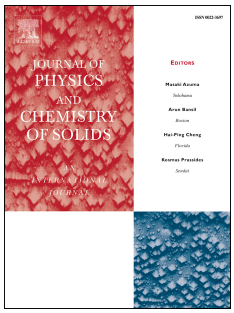

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The pressure-induced indirect to direct bandgap transition and thermoelectric response in $SrTiO_3$: an ab-initio study

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Abstract

In this paper, we investigate the electronic structure, optical and thermoelectric properties of the $SrTiO_3$ (STO) at a variant pressure from 0-120 GPa. The thermodynamic and structural stability has been confirmed from the enthalpy of formation and tolerance factor. The implementation of pressure has been found to shift the indirect band gap to direct gap at 107 GPa to tune the optical and thermoelectric properties. The optical behavior of STO has been discussed by the dielectric constant and refraction of light in the visible and ultraviolet region. Furthermore, the thermoelectric behavior has been explored by investigating the electrical conductivity, thermal conductivity, See-beck coefficient and power factor. The thermal efficiency has been elaborated from the figure of merit, which shows the studied materials are highly valuable for energy device applications.

Key Words:

Under-pressure ab-initio study; Direct bandgap semiconductor; Density functional theory; optical properties; Energy device applications