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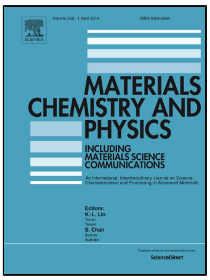

First principles study of ferromagnetism, optical and thermoelectric behaviours of AVO_3 (A = Ca, Sr, Ba) perovskites

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First principles study of ferromagnetism, optical and thermoelectric behaviours of AVO_3 (A = Ca, Sr, Ba) perovskites

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Abstract

The structural, magnetic, optical and thermoelectric characteristics of $CaVO_3$, $SrVO_3$ and $BaVO_3$ perovskite compounds computed by DFT scheme are presented. The electronic properties are computed to confirm the half-metallic ferromagnetism. The comparisons of crystal field, John Teller and the exchange energies elucidate that the electronic spins play a major role in inducing ferromagnetism. The complete set of computed optical parameters illustrate that the investigated perovskites are active for the visible and ultraviolet regions. The thermoelectric characteristics thoroughly elaborated, within the temperature range 200-800K, illustrate that the perovskites are also suitable for the energy renewable device applications.

Keywords:

Half-metallic Ferromagnetism; Density Functional Theory; optical properties; thermoelectric properties;