
Relationship between thermoelectric features and dimensionality in monochalcogenide compounds

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Description:

Proyecto asignado a través de la [Red Española de Supercomputación](#) [2].

In recent years, semiconductor materials based on chalcogenides have received great attention owing to their wide applications in numerous fields. In addition, chalcogenide elements are earth abundant, cheap and non-toxic. One of the main potential applications for chalcogenide-based semiconductor is the thermoelectricity. Although compounds here studied (concretely SnX and SnX₂ with X = S, Se, Te) have been extensively characterized, theoretical studies on the relationships between the electronic structure, dimensionality and thermoelectric features are very scarce. Herein, we propose a comprehensive study on the electronic structure and thermoelectric properties in chalcogenides-based semiconductor materials by using first-principles calculations combined with the Boltzmann transport theory.

Web:

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[1] <http://www.upm.es/> [2] <https://www.res.es/>