

Tin chalcogenides under compression: an *ab initio* study

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The class of tin compounds belonging to the Sn_xA_y family (where A is a member of the group-16 chalcogen atoms, $A=\text{S}, \text{Se}, \text{or Te}$, and, depending on tin valence, the stoichiometry $x:y$ spans the values 1:2, 1:1, and 2:3) has attracted interest as intercalation materials and for prospective optoelectronic applications [1]. At ambient conditions, the phases adopted by these materials (see e.g. [2]) display a layered arrangement and coordination that is substantially affected by the application of pressure, leading to important changes in their physical properties.

In this work, and as part of an ongoing comprehensive study of this class of compounds, we will present mainly theoretical results on trends followed by tin chalcogenides family members under compression, including a study of the structural evolution of the phases, their vibrational properties and Raman and infrared activity, along with energetics, stability, and discussion of the electronic structure.

This theoretical study has been carried out within the *ab initio* framework of the density functional theory (DFT), using the projector augmented-wave (PAW) scheme as implemented in the VASP computational code [3]. We have investigated the effects of different levels of approximation made in the DFT calculations for the treatment of the exchange-correlation term and the inclusion in the valence (vs. freezing in the core) of semicore d electrons. Corrections to the total energy due to van der Waals interactions of the layered structures were also taken into consideration and their effect analysed [4]. For the study of the vibrational properties of the phases the method of finite displacements on a supercell was used [5]. We provide a picture of the effect of pressure on bonding and electronic structure, with a focus on the analysis of the changes on the electronic localization and its correlation to the observed structural changes.

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