First Principles calculations of SnS_2 layered semiconductor, taking into account the Van der Waals interactions.

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Abstract

Layered semiconductors of the type MX, (X =chalcogen) are considered promising alternative materials for solar energy conversion. The *Van der Waals* cleavage plane (0001) of layered semiconductors as SnS_2 is characterized by hexagonal arrays of close packed chalcogenide ions which are covalently bound within X-M-X sandwiches. This is an ideal substrate to study fundamental aspects of the metal/semiconductor interaction as the perfect (0001) plane is considered to be free of surface states and intercalation of adsorbed metals may occur in stoichiometric amounts. In photovoltaic application the doped semiconductors plays a major roll, and one of the layered semiconductors studied is SnS_2 which have been considered as a precursor of intermediate band materials (IBM) doped with vanadium [1].

SnS_2 structure consists of sheets of tin atoms in the basal plane octahedrally coordinated between close packed sheets of sulphur atoms. The three-atomic-layer sandwich is repeated in the c direction. SnS_2 can exist in a number of different polytypes where the stacking sequences of these sandwiches vary. The simplest structure 2H (Ramsdall notation) has a stacking sequence, $A\gamma B\text{-}A\gamma B$ where the Greek letter represents the metal atom. There is one layer, and one molecular unit per unit cell. The 4H structure has a stacking sequence $A\gamma B\text{-}C\gamma D$ It has two layers and two molecular units per unit cell. The **a** lattice parameter is the same and the ***c*** lattice parameter approximately doubled with respect to the 2H structure. [2]

In this work we study the structural disposition of the most important polytypes of this layered material, the named 2H and 4H using the interatomic *Van der Waals* interactions in our theoretical calculations. We study the use of two theories in SnS_2 layered material, the Grimme [3] dispersion correction that is applied after each autoconsistent PBE electronic calculation and the self-consistent Dion functional optimized for solids by Michaelides et al. [4]

The Grimme approach, intrinsically possesses a semiempirical implementation which take into account the *Van der Waals* radius and the electrostatic interaction between the layers. The self-consistent functional, on the other hand, uses a complete theoretical approach. In this work the results demonstrates the enhancement of the geometric parameters by the use of the *Van der Waals* interactions in agreement with the experimental values when either Grimme or the new functionals are used.

References

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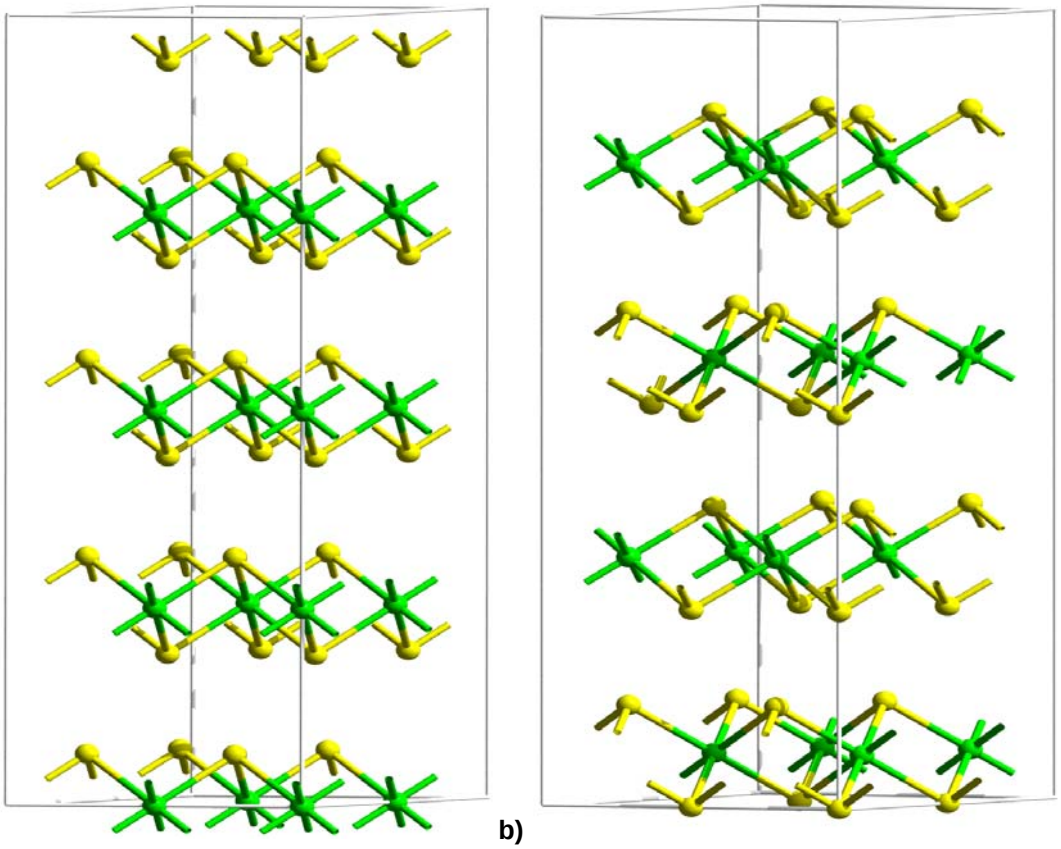
Figures



a) **b)**

Fig 1 – SnS2 polytypes supercells of b) 2H and b) 4H, where the differences on the pile stacking of the layers can be observed.