Ab-Initio calculations including Van der Waals interactions: the SnS_2 layered material.

Y. Seminóvski[1,*], P. Palacios[1,2], R. Grau-Crespo[3], P. Wahnón[1]

[1]Universidad Politécnica de Madrid, Grupo de Cálculos Cuánticos, ETSI Telecomunicación, Ciudad Universitaria s/n. C.P. 28040 Madrid, Spain
[2] Universidad Politecnica de Madrid, Dpt. FQAT Aeronautica, Ciudad Universitaria, 28040, Madrid, Spain
[3]University College London, Chemistry Department, address, country

Tin disulfide SnS_2 was recently proposed as a high efficiency solar cell precursor [1]. The aim of this work is a deep study of the structural disposition of the most important polytipes of this layered material, not only describing the electronic correlation but also the interatomic Van der Waals interactions that is present between the layers.

The two recent implementations to take Van der Waals interactions into account in the VASP code are the self-consistent Dion *et al.* [2] functional optimized for solids by Michaelides *et al* [3] and the Grimme [4] dispersion correction that is applied after each autoconsistent PBE electronic calculation.

In this work these two methods are compared with DFT PBE functional. The results we will presented at this Conference, demonstrates the enhancement of the geometric parameters by the use of the Van der Waals interactions in agreement with the experimental values.

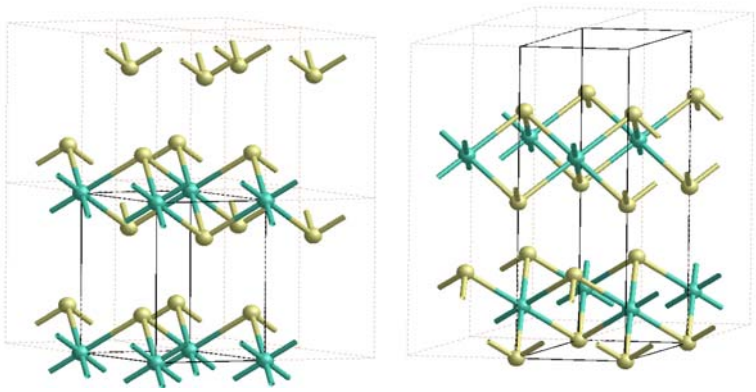

Fig. 1- SnS2 polytipes a) SnS_2-2H b) SnS_2-4H

[1] P. Wahnón et al, Phys. Chem. Chem. Phys., 2011, **13**, 20401-20407
[2] M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, and B. I. Lundqvist, Phys. Rev. Lett. **92**, 246401 (2004).
[3] J. Klimeš, D. R. Bowler, and A. Michaelides, Phys. Rev. B **83**, 195131 (2011).
[4]S. Grimme, J. Comp. Chem. 27, 1787 (2006).