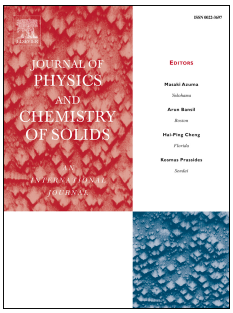
Accepted Manuscript



Structural and electronic properties of SnS_2 stacked nanosheets: An *ab-initio* study

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PII: S0022-3697(17)32517-9

DOI: 10.1016/j.jpcs.2018.04.026

Reference: PCS 8542

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 11 January 2018

Revised Date: 29 March 2018

Accepted Date: 19 April 2018

Please cite this article as: H.B. Mabiala-Poaty, D.H. Douma, B. M'Passi-Mabiala, R.E. Mapasha, Structural and electronic properties of SnS_2 stacked nanosheets: An *ab-initio* study, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.04.026.

Structural and electronic properties of SnS_2 stacked nanosheets: An *ab-initio* study

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Abstract

We present an *ab-initio* study of the structural and electronic properties of SnS_2 stacked nanosheets using the standard LDA and GGA functionals as well as the newly developed variants of the non-local van der Waals (vdW) exchange correlation functionals, namely vdW-DF-revPBE and vdW-DF2-C09. We have examined different stacking configurations of the two, three and four SnS_2 layers. The GGA-PBE functional fails to describe the interlayer binding energies and interlayer spacing of SnS_2 nanosheets, while a good agreement is observed between the calculated and available experimental values when the van der Waals corrected functionals are used, mostly the vdW-DF2-C09. It is found that the interlayer interactions in the SnS_2 films are not only vdW type but, the overlap of wave functions of neighboring layers have to be taken into account. We have observed a systematic reduction in the band gap with the increase in the number of stacked layers. This can be another way of controlling the band gap of SnS_2 nanosheets as required for electronic devices.

Keywords: DFT, nanosheets, van der Waals exchange correlation functionals, electronic structure, 2D materials, SnS_2.