Charge transfer in misfit layer compounds: the case of SnS–SnS_2 and LaS–TaS_2

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Nowadays, materials scientists are interested not only in atomically thin monolayers, but also in various multi-layered structures, which could be built up from the same or from different two-dimensional monolayers. The latter case corresponds to the class of *mixed layered compounds*. Since the lattice dimensions of different layers need not be commensurate with each other, the resulting structures are usually characterized by a lattice mismatch between two (or more) layers. These systems are called *misfit layer compounds* [1].

Here we present a study of two misfit layer compounds, namely SnS–SnS_2 [2] and LaS–TaS_2 [3] (Fig. 1), as typical examples for different magnitudes of charge transfer and strength of the interlayer interaction. We have employed a density-functional theory-based approach to calculate structural, energetic, and electronic properties of these structures [4]. We have examined the differences between individual layers, combined double-layer systems and periodically stacked bulk structures. We have shown how the chemical constitution of the sublayers affects the interlayer interactions: these may be weak non-bonding van der Waals forces which dominate interlayer interactions in SnS–SnS_2 or a strong interaction related to a remarkable charge transfer between the layers as found in LaS–TaS_2. For a better visualization of a frontier orbital overlap of two monolayers in each case, we studied the densities of states of these layers (schematically shown in Fig. 2). From these diagrams, it becomes clear that an overlap of one layer's HOCO with the other layer's LUCO only occurs in the LaS–TaS_2 system.

References

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[2] G. Radovsky, R. Popovitz-Biro, R.Tenne. *Chem. Mater.*, ***24***, 3004–3015 (2012).
[3] A. Jobst, S. van Smaalen. *Acta Cryst.B*, ***58***, 179–190 (2002).
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Figures

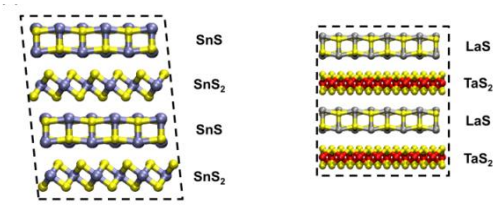

Figure 1: The structures of misfit layer compounds SnS–SnS_2 and LaS–TaS_2.

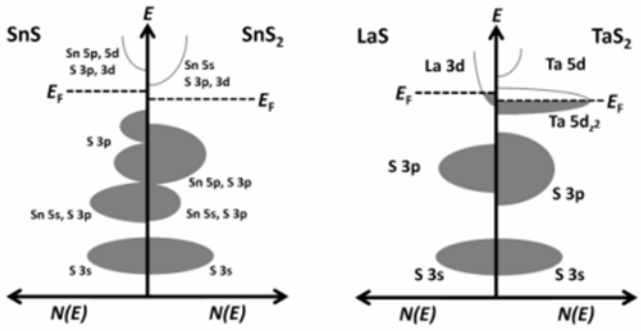

Figure 2: The densities of states for SnS–SnS_2 and LaS–TaS_2.