Hybrid functional study of laminar PbS

PbS is a narrow gap semiconductor with interesting electronic properties owing to the large spin-orbit interaction. Both the intrinsic structure and nanoscale effects (in quantum dots) are complex and potentially useful for applications[1, 2, 3]. Thin sheets of PbS, consisting of only a few atomic planes, can be fabricated and show very interesting confinement effects in the electronic structure. We would like to be able to describe these confinement effects by doing ab-initio calculations for the electronic structure of the bulk as well as periodic planar structures, starting at single layers and proceeding to realistic thicknesses.

The conventional exchange-correlation functionals in DFT, specifically the local density approximation and generalized gradient approximation, give very poor descriptions of PbS – giving a metallic instead of semiconducting groundstate – and advanced methods are needed. Hybrid functionals, which use a combination of DFT-functionals and exact exchange have been shown to be very accurate for this material[4]. Calculations using hybrid functionals will be conducted using the VASP ab-initio code[5]. The effect of surface passivation, the satisfaction of dangling bonds by hydrogen, should also be studied in the layered case.

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