Two-Dimensional Materials Beyond MoS_2

Thomas Heine, Pere Miró, Mahdi Ghorbani-Asl

Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany
t.heine@jacobs-university.de

Abstract
The development of small electronic components is fundamental in our highly technology dependent society. Currently, the electronic industry is rapidly approaching the limit of silicon-based complementary metal-oxide-semiconductor (CMOS) technology. In consequence, the development of new technologies to replace silicon has rapidly become a hot topic not only in the academic community but also in industry. This new Holy Grail of electronic materials has to perform better than silicon at smaller scales (>10 nm) and if possible add new functionalities for electronic devices such as flexible electronics. In this direction, single layer transition metal chalcogenides (TMCs) have recently emerged in nanoelectronics, although the study of layered TMCs beyond MoX_2/WX_2 is still incipient.

The electronic structure of nickel, palladium and platinum TMDs with sulfur, selenium and tellurium as the chalcogenide were investigated via periodic density functional theory calculations. All disulfide monolayers are indirect band gap semiconductors with band gaps of 0.5, 1.1 and 1.7eV for NiS_2 PdS_2 and PtS_2, respectively. The MSe_2 and MTe_2 analogues present significantly smaller band gaps and can even become semimetallic or metallic materials. Under mechanical strain these MX_2 materials become quasi-direct band-gap semiconductors. The mechanical-deformation and electron-transport properties of these materials indicate their potential application in flexible nanoelectronics [1].

In the second part, we will present the electronic properties of the most interesting 2D materials beyond graphene, in particular of all transition metal chalcogenides and halides. We concentrate on the dependency of the electronic band gap on the number of layers (magnitude and character), and the effective hole and electron masses [2].

References

[1] P. Miró, M. Ghorbani-Asl, T. Heine, Angewandte Chemie Intl. Ed. (2014) in press.
[2] P. Miró, M. Audiffred, T. Heine, Chem. Soc. Rev. (2014) submitted.

Figures

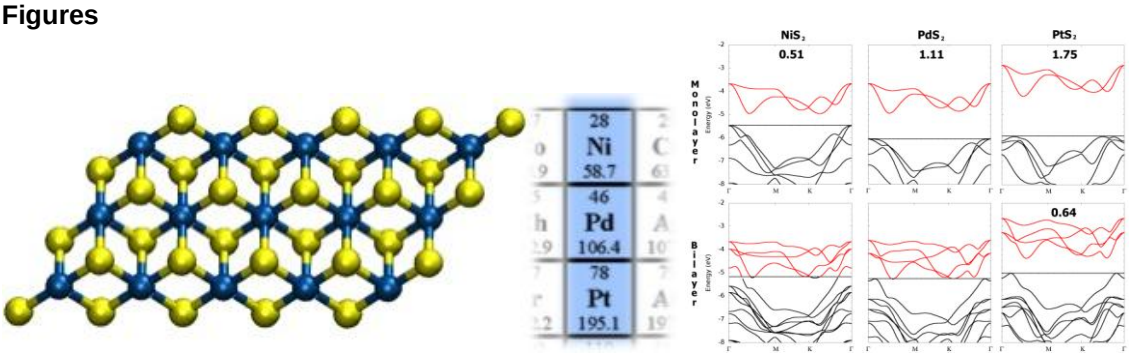

Figure 1. Left. Structure of TX_2, T=Ni, Pd, Pt, X=S, Se, Te. Right: band structure of these materials a monolayer (top) and bilayer (bottom). Note that PdS_2 is semiconducting as monolayer, but metallic as bilayer.