Trans2DTMD: Theoretical investigation of electronic transport in functionalized 2D transition metal dichalcogenides

Main area: Computational modeling of devices and systems
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Abstract

Metallic transition metal dichalcogenide (TMD) monolayers are promising ultrathin materials which have the potential to complete the range of graphene-related materials by offering tunable metallic phases with strong spin-orbit coupling. Many of them can be achieved by small structural deformations and doping of Group VI TMDs and could thus be used as electrode materials within a single monolayer, resulting in a very low contact resistance. Experimental study of metallic TMDs is difficult as these phases are often metastable or rely on very subtle structural modifications.

Thus, a careful theoretical investigation is imperative before complex experimental studies should be pursued.

This consortium will investigate metallic TMD structures, including intrinsically metallic phases, metastable metallic phases, and external factors to trigger semiconductor-metal transitions such as doping, defects and strain. Special attention will be given to spin-orbit splitting and ways to control them. Computer simulations will range from band-structure calculations of small unit cells to rather complex systems, including heterostructures, doped and defected systems up to grain boundaries. Conclusions on the suitability of these materials in practical application will be further confirmed by explicit transport calculations and device simulations. While most calculations can be carried out using state-of-the-art software, some method developments are necessary and will be carried out here. Numerical methods that scale linearly with the system size, O(N), will be developed by using a polynomial expansion of the components of the conductivity tensor. These will allow for simulations of large unit cells in the presence of disorder and the calculation of spin- and valley-dependent contributions. It will become therefore suitable to describe the Spin and Valley Hall effects in realistic models of TMDs.

Besides metallic TMDs we will also investigate the possibility of functionalizing semiconducting TMDs for spintronics applications. The possibility of creating the two-dimensional equivalent of the dilute magnetic semiconductor will have a strong impact on spintronics research. By doping with magnetic transition metals, we will investigate the possibility of inducing a tunable magnetic phase transition. On a similar note, we will model the coupling of 2D materials with ferromagnetic contacts and study the effect of disorder and spin-orbit interactions on the performance of such contacts in spintronic devices.

The consortium will maintain its excellent relationship to various members of the FLAGSHIP Graphene core project.

Consortium

Francois Peeters - University of Antwerpen - Belgium - Funded by: FWO - (Coordinator)
Thomas Heine - Jacobs University Bremen - Germany - Funded by: DFG
Paul J. Kelly - Universiteit Twente - Netherlands - Funded by: Partner not requesting funding
Angel Rubio - Universidad del País Vasco - Spain - Partner not requesting funding
Gotthard Seifert - Technische Universität Dresden - Germany - Partner not requesting funding