Quantum transport in TMDs lateral heterojunctions

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Novel prospects for the quasi-perfect assembly of lateral and vertical heterostructures have been recently proposed by combining layers of two-dimensional materials (2DMs)[1]. Those 2DMs-based heterostructures are characterized by dangling-bond free surfaces and atomically abrupt interfaces[2]. Such features combined with the large number of existing 2DMs offer opportunities for inventive device engineering at the atomistic scale.

From a quantum mechanical perspective, the fundamental properties of lateral heterojunctions (LHs) are determined by the nature of the adjacent 2DMs, the long-range coupling between the layers and the interface local electronic characteristics.

In this research, we present an investigation of multiple LHs composed of transition metal dichalcogenides (TMDs) such as MoS_2, WS_2, $MoSe_2$ and WSe_2.
First, density functional theory (DFT)[3] is used to explore the electronic structures (band alignment, charge exchange, ...) of supercells formed by two TMDs. Interestingly, dispersive bands related to electronic states at the interface are observed.
Afterwards, DFT and tight-binding techniques[4] based on Green's function methods are applied to investigate electronic transport through the junction (see Fig.1). The resulting conductances are found to depend on the TMDs electronic structures matching and on scattering ensuing from the junction (see Fig.2).

The results presented in this research intend to answer to the lack of characterization of TMDs-based LHs which represent an enabling device engineering technology for next-generation electronics .

References

[1] Iannaccone G., et al., Nature Nanotechnology **13.3** (2018): **183**.
[2] Zhang Ch., et al., Nature Nanotechnology **13.2** (2018): **152**.
[3] openmx-square.org/
[4] inac.cea.fr/L_Sim/TB_Sim/; zerothi.github.io/sisl/docs/latest/

Figures

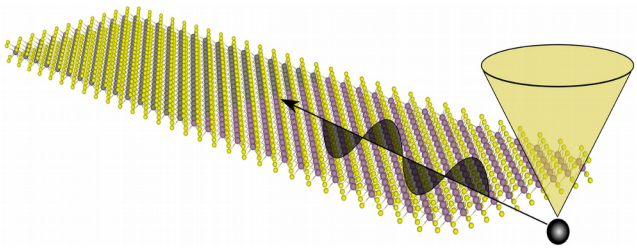

Figure 1. Modelling quantum transport through lateral heterojunction. Charge carriers are injected in TMD_1 and collected in TMD_2.

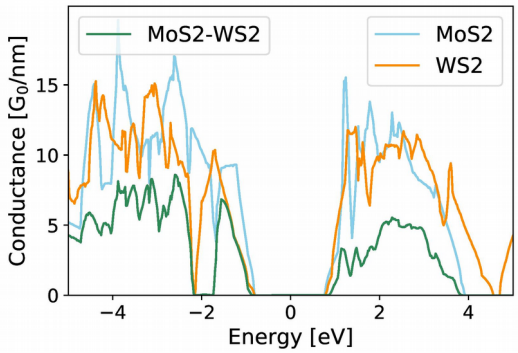

Figure 2. Zero-bias total conductance per unit length through a MoS_2-WS_2 junction as a function of energy. The total transmission (green) is limited by the lowest conductance between pristine MoS_2 (blue) and WS_2 (orange). Local scattering decreases conductances whereas an electronic structures mismatch leads to a transport gap.