2D Materials and Device Modelling: From Theory to Applications

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Two-dimensional (2D) materials and in particular transition metal dichalcogenides (TMDCs) are widely perceived as promising candidates to replace Si at the core of future logic devices, especially since the recent adoption of nanosheet transistors. The 2D technology has however not yet reached its maturity: Several challenges remain to be addressed regarding the crystal quality, contact resistance, and channel interface with amorphous oxides. Technology computer aided design (TCAD) tools, which have been used in the semiconductor industry since the end of the 1970's, could help resolve some of these issues, provided that they capture the physics of 2D materials and devices. While transistors have undergone tremendous evolutions over the last 45 years, the physical models of commercially available TCAD tools have not varied much: The propagation of electrons is still described by the drift-diffusion equations. To accurately model 2D compounds with close to atomic dimensions, reproduce their characteristics, and predict their performance a quantum mechanical treatment of their behaviour is imperatively needed. In this presentation, I will review the methods and tools that we have developed to simulate 2D devices [1,2]. After a short description of the physical models we implemented, the focus will be on the calculation of the "current vs. voltage" characteristics of transistors based on TMDCs and novel 2D materials, on the evaluation of their carrier mobility, on the investigation of contact resistances, on the influence of defects, on the role of electron-phonon scattering, and on the efficiency of light-matter interactions. These applications will be illustrated with a few simulation examples (see figure below).

References

[1] C. Klinkert, A. Szabo, C. Stieger, D. Campi, N. Marzari, and M. Luisier, "2-D Materials for Ultra-Scaled Field-Effect Transistors: Hundred Candidates under the *Ab Initio* Microscope", ACS Nano, 14 (2020) 8605.

[2] A. Szabo, R. Rhyner, and M. Luisier, "*Ab-initio* simulation of single- and few-layer MoS_2 transistors: Effect of electron-phonon scattering", Phys. Rev. B, 92 (2015) 035435.

Figures

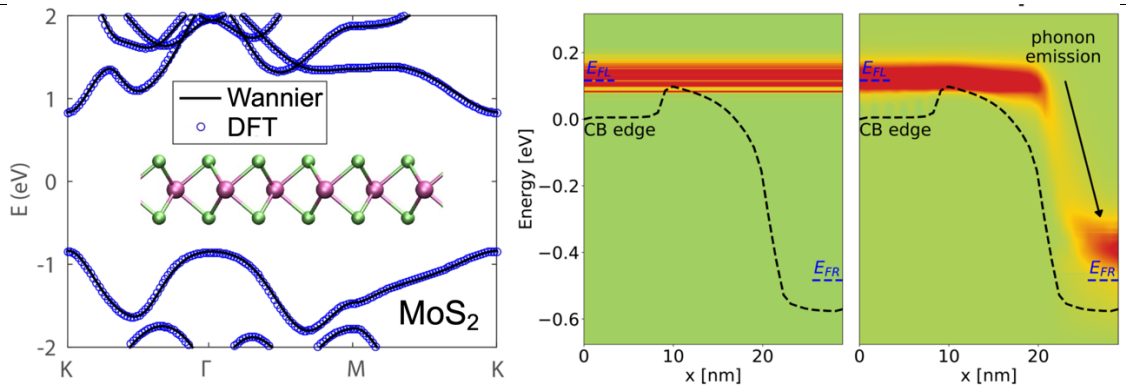

Figure 1: (left) Bandstructure of monolayer MoS_2, as computed with DFT (blue symbols) and with Wannier functions (solid line). (right) Spectral current density flowing through a monolayer MoS_2 transistor in the ballistic limit and in the presence of electron-phonon scattering. Red indicates high current concentrations, green no current. The dashed black lines refer to the CB edge.