Multi-scale approach: a versatile platform for investigating novel two-dimensional-material based device concepts

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It is nowadays more and more urgent to devise a robust and precise modeling framework able to incorporate the different 2D materials and their possible combinations in order to explore their applicability in electronics. In fact, the advent of graphene and related 2D materials has already opened the possibility to boost the transistor performance as well as to conceive novel devices by engineering new materials with tailored properties. By means of a first-principle multi-scale approach we study multiple device configurations for digital applications. The method used is articulated in three steps: density-functional-theory (DFT) calculations [1], then we pass through the expression of the Hamiltonian on the basis of a maximally localized Wannier function [2], which feeds the open-source device simulator NanoTCAD ViDES [3], based on a non-equilibrium Green's-function formalism. Specifically, we assess the performance of transistors based on InSe [3], we present lateral heterostructures made of different phases of monolayer MoS_2 [4] combining metallic and semiconducting phases to build up a Schottky diode and a lateral heterostructure FET. Then we explore different Noble TMDs materials, combining bilayer and monolayer crystals, as building block for nanoscale transistors [6]. Particular attention will be also devoted to Stanene, which has interesting features when cut into zig-zag nanoribbon. We present two different tunnel field effect transistors (TFET) using Stanene nanoribbons: a proposal of a purely one-dimensional channel TFET device [7] and a spin filter which exploits the possibility of independently tune the gap for spin up and spin down carriers with a lateral electric field [8]. Finally we present an example on how theoretical methods can help to experimental device realizations and experimental data interpretation [9].

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