Ab initio quantum transport simulation of lateral heterostructures based on 2D materials: assessment of the coupling Hamiltonians

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Lateral heterostructures based on lattice-matched 2D materials are a promising option to design efficient electron devices such as MOSFETs [1], tunnel-FETs [2] and energy-filtering FETs [3]. In order to rigorously describe the transport through such heterostructures, an ab-initio approach based on density-functional theory (DFT) is almost unavoidable due to the lack of physical characterization of the interfaces. However, due to the computational cost of including the DFT Hamiltonian describing the whole interface region in transport calculations, the matrix describing the coupling between the two materials is often approximated as the one of a single material. Here, we focus on a simple lateral heterostructure based on bi-layer/mono-layer $PtSe_2$ and compare the use of the coupling Hamiltonian matrix of the mono-layer $PtSe_2$ with the one extracted from the DFT simulation of the whole bi-layer/mono-layer $PtSe_2$ interface. To perform our self-consistent quantum transport calculations, we used the NEGF method and a reduced basis composed of unit-cell restricted Bloch functions [4]. To compute the coupling Hamiltonian between the bi- and the mono-layer PtSe2, we first performed a DFT simulation of the heterostructure sketched in Fig.1, where the dangling bonds at the interfaces are passivated by H atoms and all atomic positions have been relaxed. Hence, the plane-wave DFT Hamiltonian was transformed in the hybrid space having real-space along the x-axis and plane waves in the orthogonal directions, then, the block-matrix Hamiltonians representing the coupling between the two materials were extracted by selecting specific elements of the whole Hamiltonian and further reduced in the Bloch function basis.

Fig. 3 shows the transfer characteristics of the bi-layer/mono-layer $PtSe_2$ MOSFET in Fig.2 computed with either the coupling Hamiltonian of the mono-layer or the one extracted from the supercell in Fig 1. An appreciable difference is found at high V_{GS} values. Fig. 4 shows the comparison between the lowest conduction band (LCB) profile and the transmission probability of such a device computed with the two types of coupling matrix. The second method provides a more efficient coupling between the two materials and consequently a larger transmission. A similar analysis can be extracted from Figs. 5-6 showing the local density of states at high V_{GS}.

[1] G. Iannaccone et al. Nat. Nanotechnol. **13**, 183–191 (2018).

[2] J. Choukroun et al., Nanotechnology **30**, 025201 (2018).

[3] E. Marin et al., ACS Nano, **14**, 2, 1982-1989 (2020).

[4] M. G. Pala et al., Phys. Rev. B., **102**, 045410 (2020).

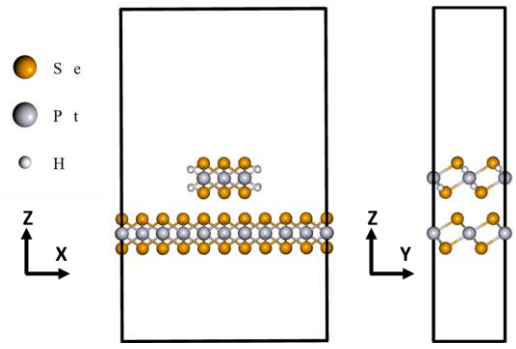

Fig.1: Sketch of the orthorhombic supercell used to simulate the monolayer/bilayer $PtSe_2$ lateral heterostructure. The dangling bonds at the interfaces were passivated with H atoms. Unit-cell vectors: a_x=11.136 Å, a_y=6.429 Å, a_z=30.0 Å.

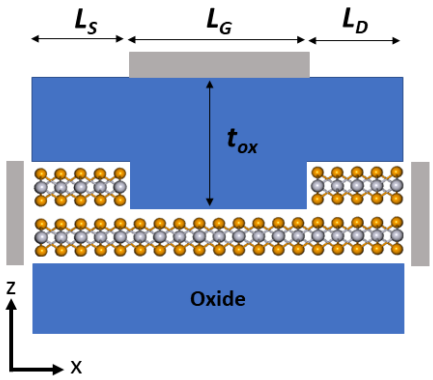

Fig.2: Sketch of the bi-layer/monolayer $PtSe_2$ single-gate MOSFET. Geometrical parameters: L_S=L_D=11nm, L_G=15nm, t_{ox}=2nm. The bi-layer is n-doped with a concentration of N_D=5x10^{13}cm^{-2}.

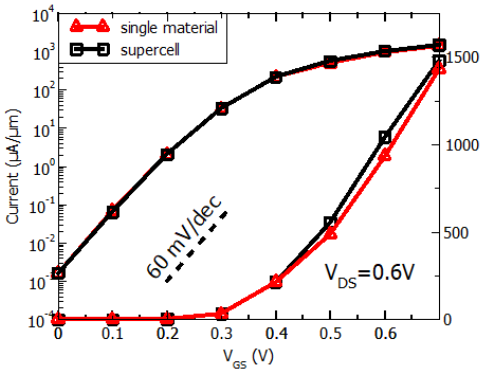

Fig.3: Transfer characteristics of the device in Fig. 2 computed by using the coupling matrix of the single material (mono-layer $PtSe_2$) and the one extracted from the supercell in Fig. 1.

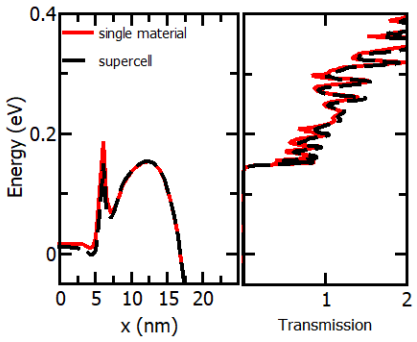

Fig.4: Conduction band profile and transmission probability computed at V_{GS}=0.5V by using the coupling matrix of the single material and the one extracted from the supercell in Fig. 1.

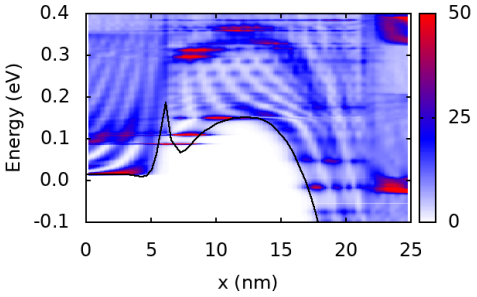

Fig.5: Lowest CB profile along the transport direction (black line) and LDOS of the device in Fig. 2 simulated with the coupling matrix of the monolayer. V_{GS}=0.5V.

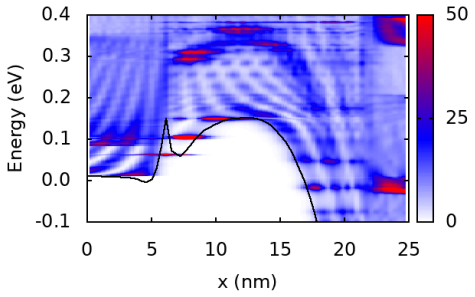

Fig.6: Same as in Fig. 5, but simulated with the coupling matrix extracted from the supercell in Fig. 1. A small difference can be detected at the interface between bi- and mono-layer (x=7 nm).