AB-INITIO SIMULATION OF PHONON-ASSISTED ELECTRON TRANSPORT IN VAN DER WAALS HETEROSTRUCTURES

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Van der Waals (vdW) heterostrures are a promising option to design innovative electron devices due to their low defect densities, large tunneling currents and optimal electrostatic control [1]. In this work, we propose a first-principles study of electronic quantum transport in a vdW heterostructure tunnel-FET sketched in Fig. 1. In order to rigorously describe the material properties and quantum phenomena governing this device, we adopted a full *ab initio* methodology, and employed a density functional theory (DFT) Hamiltonian to self-consistently solve the quantum transport equations within the non-equilibrium Green's function (NEGF) formalism by coupling them with the 3D Poisson equation [2].
We focused on the system composed by 1T-$HfSe_2$ and 1T-SnS_2, two TMDs with a type II band alignment[3] and close to type III as illustrated by Fig. 2. To include dissipative scattering due to the electron-phonon interaction in our transport calculations, we first performed density functional perturbation theory (DFPT) and found that the dominating mode is the longitudinal optical (LO) phonon mode. We approximated the Fröhlich interaction of LO polar phonons through an effective deformation potential equivalent to the scattering rate computed with the 2D model of Ref. [4]. Phonon scattering was then included in the NEGF code with local self-energies and adopting the self-consistent Born approximation (SCBA).
Figure 3 shows the computed transfer characteristics for different values of the LO phonon scattering rate. It can be noticed that a stronger el-ph interaction degrades the sub-threshold swing and moreover it can increase the on-state current. These behaviors can be explained by inspecting the spectral current shown in Fig. 4 and Fig. 5 for the off- and on-state, respectively. The former highlights the role played by phonon absorption in the overlap region in increasing the off-state current, the latter illustrates the phonon emission in the drain responsible for inter-valley scattering and consequently in a current higher than in the ballistic case.

References

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[3] S. Su et al., *J. Chem. Phys.* **146**, 064701 (2017)
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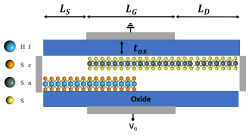

Figure 1: Sketch of the vdW Tunnel-FET with source/drain length of $L_{S/D}$=8 nm, and gate length of L_G=15 nm.

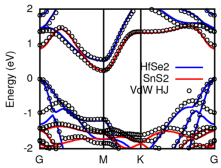

Figure 2: Band structure of 1T-SnS_2 and 1T-$HfSe_2$ and their VdW heterostructure

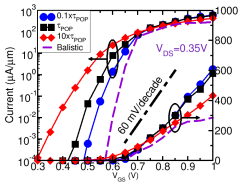

Figure 3: I-V curves for different scattering rate. V_{DS}=0.35 V.

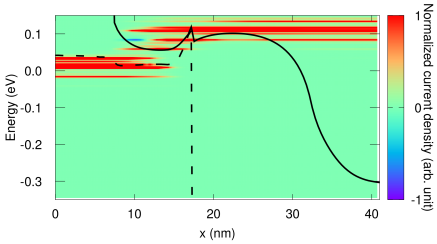

Figure 4: Spectral current density along the device in the off state.

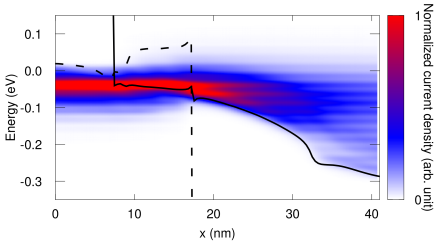

Figure 5: Spectral current density in ON state with a scattering rate at $10\times\tau_{POP}$

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