Quantum transport prediction of recombination in vertical pn junctions

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Vertical heterojunctions of a p-doped black phosphorous monolayer and n-doped MoS_2 monolayer have exhibited anti-ambipolar (AAP) behaviour [1]. Various scenarios that can lead to the AAP characteristics have been discussed, but the applied models had been semiclassical so far [2]. Given the countable number of atoms in the critical device dimensions, pronounced quantum effects such as tunnelling, confinement and interferences are expected. Therefore, in this work, the nonequilibrium Green's function method of NEMO5/Victory Atomistics is applied on electron and hole quantum transport in the BP/MoS_2 vertical heterostructure. Incoherent scattering on phonons and electron-hole recombination is included with Büttiker probe self-energies [3]. The experimental AAP characteristics are qualitatively reproduced and the mechanisms that control the effective recombination and with it the device current are assessed in high detail.

References

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Figures

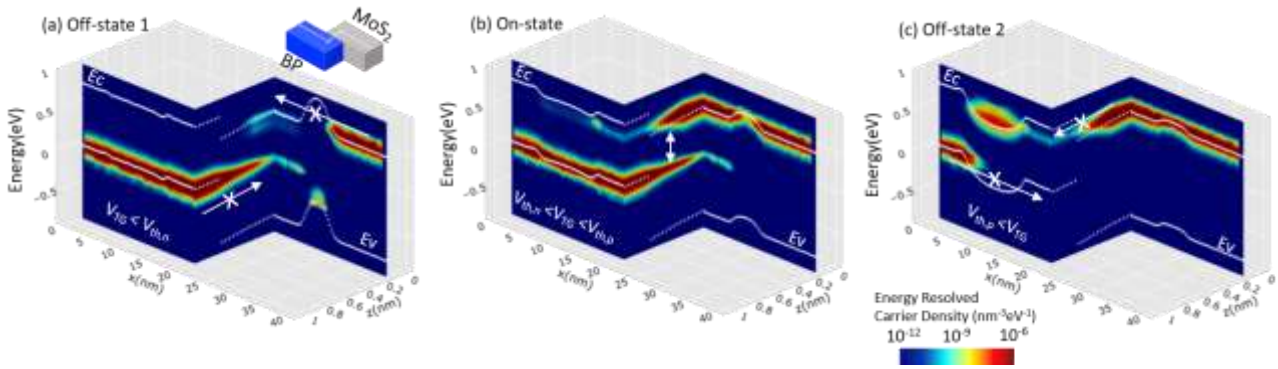

Figure 1: Quantum transport prediction of electrons and holes in the BP/MoS_2 vertical pn junction. For low (high) gate voltages, barriers in the conduction (valence) band prevent electrons (holes) to reach the interface area which creates the Off-state 1 (Off-state 2) in Fig.1 a (Fig. 1 c). This is indicated with the crossed arrows. For moderate gate voltages, electrons and holes meet at the BP/MoS_2 interface and recombine there (indicated by a double-arrow in Fig.1 b). The resulting AAP characteristics agree qualitatively with experimental data.