First-Principles Studies of Charge and Spin Transport in 2D MoS2 Junctions

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The current rate of technological evolution necessitates a greater understanding of low-dimensional materials and their physical properties. As a result of the search for improved nanoscale electronic devices, transition metal dichalcogenides have come into focus. These materials have been shown to have applications in tunneling field-effect transistor and Esaki diode devices. In doped molybdenum disulfide p-n junctions, band-to-band tunneling is the foremost contributing factor to Esaki diode behavior at low potential bias. Using the non-equilibrium Green's function approach and effective screening medium in the framework of density functional theory (NEGF +ESM+ DFT), we investigated MoS_2 mono- and bi-layer junctions. Esaki diode behavior and a negative differential resistance regime are observed in these systems. Analysis of partial density of states reveals that the current across the junction is due to interlayer band-to-band tunneling. Finally, we discuss edge effects and edge state termination.