Negative Differential Resistance in MoS2 Esaki Diodes

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MoS_2 is a two dimensional semiconducting system with valued potential as a programmable material. In addition to its direct bandgap in a single layer, an external electric field allows for a direct bandgap transition in bilayer configuration, which raises the prospect of tunneling current in nanojunctions. Incorporating a first principles approach via DFT+NEGF, we analyze the electronic properties of both planar and interlayer MoS_2 p-i-n junctions. We display density of states alongside the IV characteristics of our junctions, comparing band alignment at biases of interest. We directly demonstrate interlayer band to band tunneling by comparing the band structure of the electrodes and the transmission function of our interlayer junction. Finally, we discuss edge termination and the resultant effect on electronic structure.