

Nanoscale device design and modeling

Our Nano computational group is focusing on the fundamental understanding of the 2D/1D materials and scope of engineering on the metal semiconductor contact using different quantum computations (DFT, NEGF, MD) to boost carrier and thermal transport through the junction. They also explore different techniques of channel and dielectric engineering to enhance electrical, thermal and optical properties of 2D materials (TMDs and Xenes) and their hetero structure devices. Atomistix Tool Kits (ATK) and Vienna Ab initio Simulation Package (VASP) are being used for different quantum computation.