Contact Engineering and Device Performance Analysis of 1T-phase TMD (such as HfS_2) with Metallic/Semi-metallic Contacts Using Quantum ATK and TCAD Simulations.

Abstract

Two-dimensional transition metal dichalcogenides (TMDs) have emerged as leading silicon-alternative channel materials due to their atomic thickness, tunable bandgaps, and excellent electrostatic control. While the semiconducting 2H-phase TMDs such as MoS_2 dominate transistor channel applications, 1T-phase TMDs such as HfS_2 have recently emerged as superior alternatives due to their higher theoretical electron mobilities and favorable thermodynamic stability. 1T-HfS_2 exhibits high electron mobility and moderate band gaps suitable for logic applications, whereas MoS_2 suffers from low electron mobility.

Despite these intrinsic advantages, device performance is severely limited by extrinsic factors, most notably the high contact resistance at the metal–semiconductor interfaces of source and drain terminals of a transistor. When a 3D metal is deposited onto a 2D semiconductor, chemical bonding often damages the delicate 2D lattice, and metal-induced gap states (MIGS) cause Fermi-level pinning (FLP), resulting in a significant Schottky barrier and degraded device performance. Recently, semi-metals (such as bismuth) and metallic TMDs have shown theoretical capability to suppress MIGS and alleviate FLP in certain 2H-TMDs, yielding low contact resistance. However, the interfacial physics of 1T-phase TMDs (such as HfS_2 and ZrS_2) remains largely unexplored. This research gap is critical because without low-resistance Ohmic contacts, the intrinsic high mobility of 1T-phase TMDs cannot be translated into superior device performance.

This project will address that gap by establishing a multi-scale modeling pipeline to screen metallic and semi-metallic electrodes, quantify contact parameters, and simulate device-level transport. Using QuantumATK, which integrates density functional theory (DFT) with non-equilibrium Green's functions (NEGF), we will accurately calculate the atomistic electronic structure and quantum transport at the metal/1T-TMD interface, extracting band alignment, charge transfer, Schottky barrier height, and specific contact resistivity. These quantum-derived parameters will then inform continuum-level simulations in Sentaurus TCAD to model realistic 2D FET I–V characteristics, ON/OFF current ratios, subthreshold swing, and contact-limited performance metrics. By bridging atomistic interface physics with device-level transport modeling, this study will identify optimal electrode–1T-TMD pairings that minimize contact resistance and maximize switching efficiency.