**Atomistic origins of low-resistance metal contacts to phase-engineered MoS2**

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In realizing high-performance electronic devices based on transition metal dichalcogenides (TMDCs), the high contact resistance at the metal-TMDC interface remains a major obstacle to overcome. Recently, the phase engineering of TMDCs has been demonstrated as a promising scheme to achieve low-resistance contacts for ultrathin TMDC transistors, but its atomistic mechanism remains unclear. Here, carrying out density functional theory (DFT) and DFT-based matrix Green’s function calculations, we systematically explore the roles of 1T MoS2|2H MoS2 and metal/1T MoS2 interfaces in lowering contract resistance for phase engineered TMDCs by considering different electrode metal species (In, Pd, Au) and the top and edge contact configurations. We demonstrate that the improved charge injection mainly results from the lower contact resistance of the extrinsic metal|1T MoS2 interface rather than the intrinsic 1T MoS2|2H MoS2, counterpart.