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First-principles study of Schottky and Ohmic contacts at metal/two-dimensional semiconductor interface. YANWEN CHEN, Tsinghua Univ, YUANCHANG LI, National Center for Nanoscience and Technology, JIAN WU, WENHUI DUAN, Tsinghua Univ — The quality of electrical contact is as important as the semiconductor itself to the performance of the entire devices, which becomes particularly crucial in the two-dimensional (2D) cases. Using first-principles calculations, we investigate the interfacial properties of single-layer titanium trisulfide (TiS_3) and metal contacts in detail, including the geometry, bonding, electronic structure, charge transfer and local potential. We observe that the contacts with Au(111), Ag(111), Al(111), and Cu(111) are of Schottky type with the barriers of 2.15, 1.67, 1.55, and 0.84 eV while that with Sc(111) is of a low-resistance Ohmic type, originating from the strong hybridization between TiS_3 and Sc(111). In comparison with calculated results of other five typical 2D semiconductors (namely, graphene, MoS_2, WS_2, $MoSe_2$ and black phosphorene), we reveal an interesting dependence of the contact type on the separation d between metal and 2D semiconductor.

Yanwen Chen
Tsinghua Univ

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