First-principles analysis of MoS$_2$/Ti$_2$C and MoS$_2$/Ti$_2$CY$_2$ (Y=F and OH) all-2D semiconductor/metal contacts

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Semiconductors/metals heterostructures play a key role in modern electronic and photonic devices [1], being more crucial than the semiconductors themselves. Particularly, coherent and passivated interfaces govern the properties of high mobility transistors, solid state lasers, light emitting devices, and solar cells, since interfacial defects can severely degrade the performance [2]. Single-layer transition metal dichalcogenides (TMDCs), especially monolayer MoS$_2$, exhibit many promising prospects in electronics and optoelectronics due to their exotic electronic, optical, mechanical, chemical, and thermal properties, as compared to their bulk counterparts [3-6]. Integration of MoS$_2$ with other 2D materials to form 2D hybrid systems can give rise to remarkable electronic properties, and thus attract increasing interest [7, 8]. Very recently, new families of 2D graphene-like carbides and carbonitrides, so-called MXenes, have been synthesized from layered M$_{n+1}$AX$_n$ (n=1, 2, and 3) [9, 10], in which A represents elements mainly from groups IIIA and IVA. These materials display not only structural similarity to graphene but also show a high electrical conductivity, which may allow enhancing TMCD electronic devices by forming MoS$_2$/MXenes heterojunctions.

First-principles calculations are used to explore the geometry, bonding, and electronic properties of MoS$_2$/MXenes semiconductor/metal contacts, taking Ti$_2$C and Ti$_2$CY$_2$ (Y=F and OH) as prototypes [11]. The structure of the interfaces is determined for the first time. The three kinds of interfaces, MoS$_2$/Ti$_2$C, MoS$_2$/Ti$_2$CF$_2$, and MoS$_2$/Ti$_2$C(OH)$_2$, can be divided into two classes according to the calculated energetics. Strong chemical bonds form in MoS$_2$/Ti$_2$C, while a much weaker interaction (that is not sensitive to the specific geometry) is found in the latter two interfaces. The metal induced states significantly modify the electronic structure of MoS$_2$ in the case of MoS$_2$/Ti$_2$C. The fact that a metallic character emerges shows that deposition of Ti$_2$C on MoS$_2$ can lead to conductive MoS$_2$. In both the MoS$_2$/Ti$_2$CF$_2$ and MoS$_2$/Ti$_2$C(OH)$_2$ interfaces the semiconducting nature is preserved for the physisorbed MoS$_2$. The bond alignment implies weak and strong $n$-type doping of the MoS$_2$ in MoS$_2$/Ti$_2$CF$_2$ and MoS$_2$/Ti$_2$C(OH)$_2$ with corresponding $n$-type Schottky barrier heights of 0.85 and 0.26 eV. The MoS$_2$/Ti$_2$CF$_2$ interface is found to be close to the Schottky limit with negligible charge transfer at the interface. At the MoS$_2$/Ti$_2$C(OH)$_2$ interface a 2.50 eV discontinuity between the vacuum levels on the two sides of the interface indicates that the barrier in this case is mainly due to the interface dipole induced by charge rearrangement.
References


Figures

Side views of the six non-equivalent stacking patterns of the MoS$_2$/Ti$_2$C(OH)$_2$ interface.

Energy level alignments of MoS$_2$/Ti$_2$CF$_2$ and MoS$_2$/Ti$_2$C(OH)$_2$ heterostructures.