First-principles analysis of MoS_2/Ti_2C and $MoS2/Ti_2CY_2$ (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_2C and Ti_2CY_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_2C, MoS_2/Ti_2CF_2, and $MoS_2/Ti_2C(OH)_2$, can be divided into two classes according to the calculated energetics. Strong chemical bonds form in MoS_2/Ti_2C, 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_2C. The fact that a metallic character emerges shows that deposition of Ti_2C on MoS_2 can lead to conductive MoS_2. In both the MoS_2/Ti_2CF_2 and $MoS_2/Ti_2C(OH)_2$ 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_2CF_2 and $MoS_2/Ti_2C(OH)_2$ with corresponding *n*-type Schottky barrier heights of 0.85 and 0.26 eV. The MoS_2/Ti_2CF_2 interface is found to be close to the Schottky limit with negligible charge transfer at the interface. At the $MoS_2/Ti_2C(OH)_2$ 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

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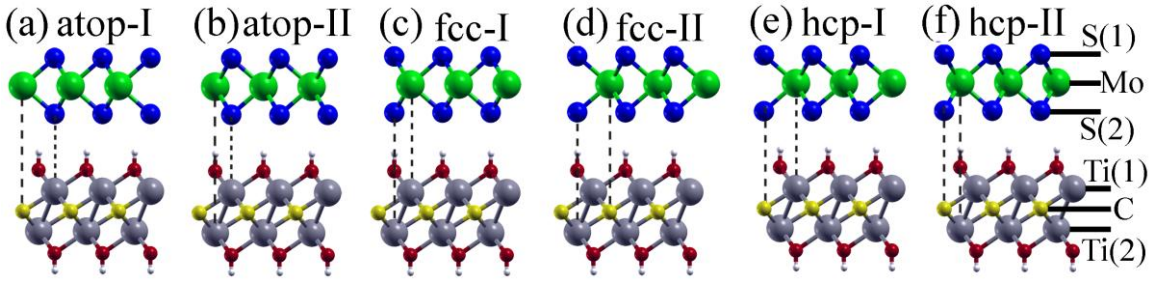
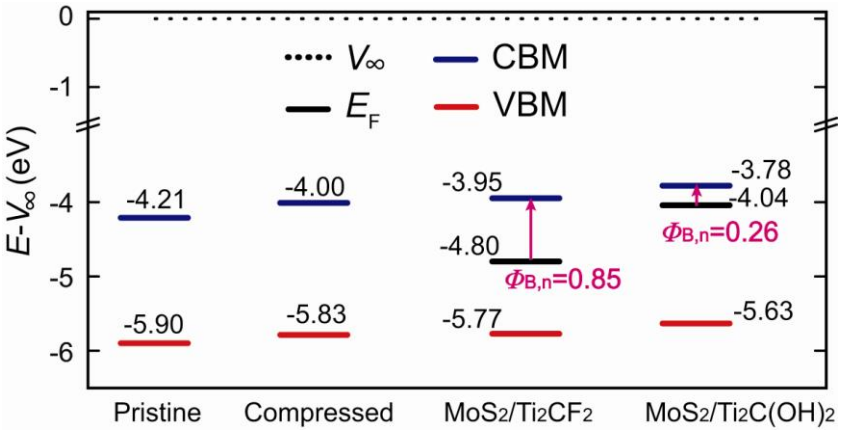
Figures



Side views of the six non-equivalent stacking patterns of the $MoS_2/Ti_2C(OH)_2$ interface.



Energy level alignments of MoS_2/Ti_2CF_2, and $MoS_2/Ti_2C(OH)_2$,heterostructures.