Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Designing high performance metal-mMoS$_2$ interfaces by two-dimensional insertions with suitable thickness

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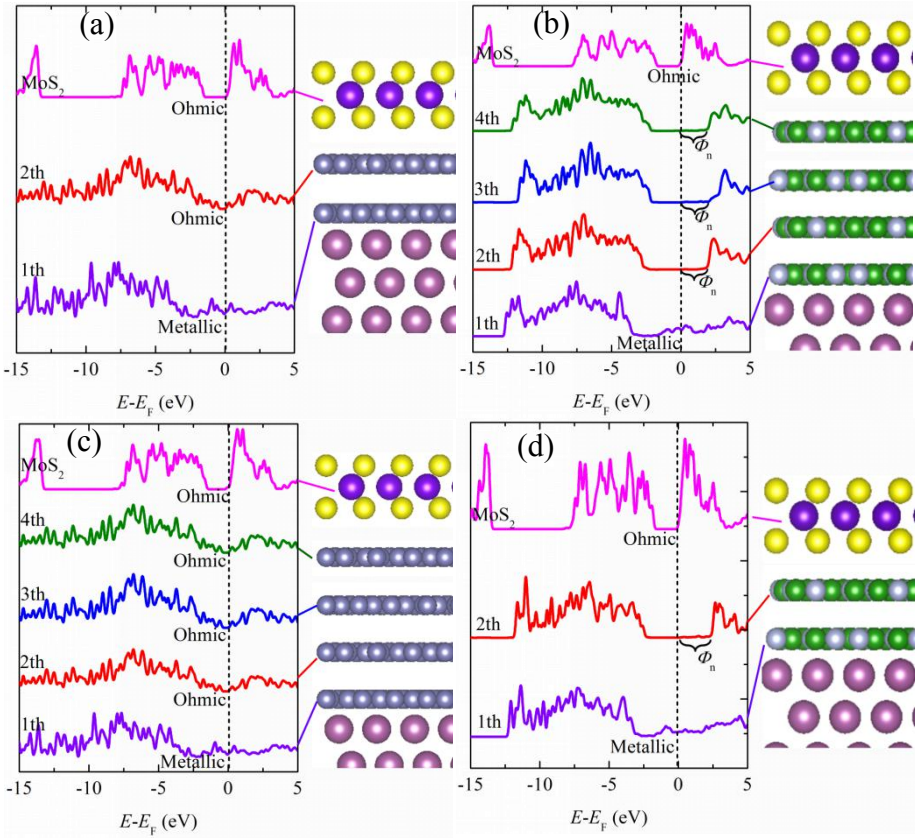

Figure S1.projected layer density of states of (a) Sc/2g-mMoS$_2$, (b) Sc/2BN-mMoS$_2$ interfaces, (c) Sc/4g-mMoS$_2$, and (d) Sc/4BN-mMoS$_2$ interfaces, respectively. The contact character of each layer is marked in these plots.

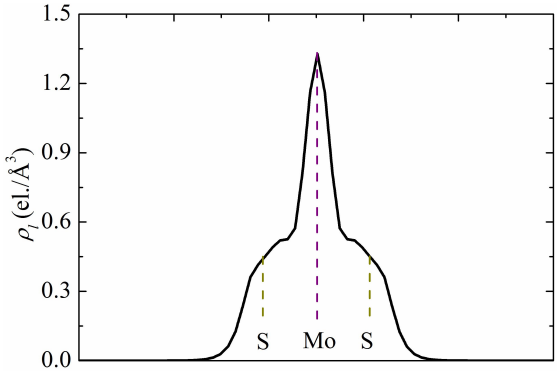

Figure S2. Plots of the plane-averaged charge density along the z-direction normal to the surface of isolated mMoS_2.

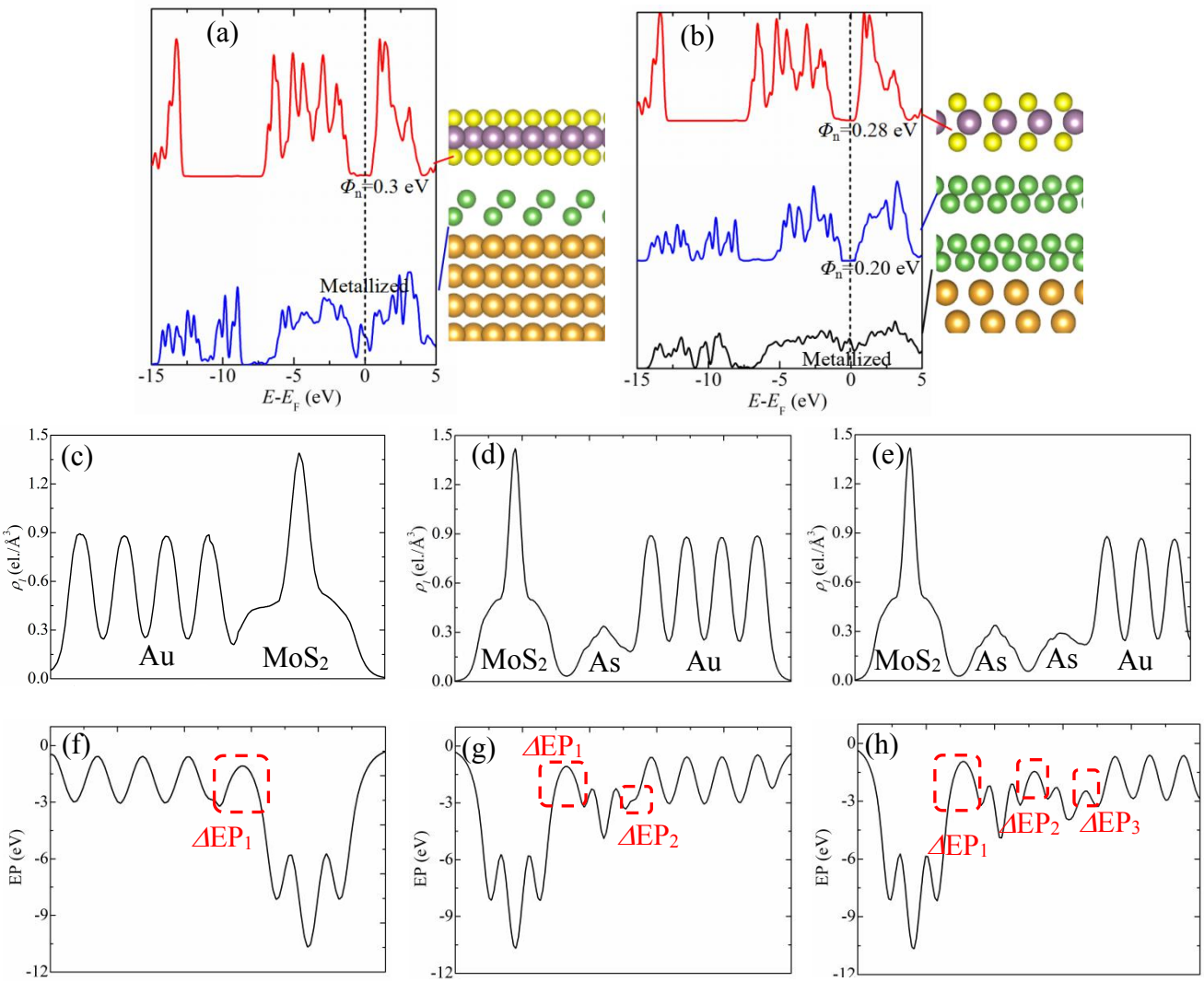

Figure S2. Projected layer density of states of (a) Sc/1As-mMoS_2 interface and (b) Sc/2As-mMoS_2 interface. The right panel of each figure is the optimized Sc/1As-mMoS_2 and Sc/2As-mMoS_2 interfaces in side view. As represents the Arsenene. Electronic structures of Sc-mMoS_2 interfaces systems: (c, f) Au-mMoS_2 interface, (d, g) Sc/1As-mMoS_2 interface, (e, h) Sc/2As-mMoS_2 interface. The up panels are the average electron density $<\rho_l>$, which is the average electron density value in the x-y planes parallel to the z axis. The bottom panels are average effective potential (EP), which is the average electrostatic potential in the *x*-*y* planes normal to the *z* axis. ΔEP represents the tunneling barrier.

Previous studies [10, 19, 26] have reported that the Schottky barrier of Au-mMoS_2 interface is about 0.69 eV. Upon inserting As into the Au-mMoS_2 interfaces, the Schottky barriers of Au-mMoS_2 interfaces significantly reduce to 0.28~0.30 eV, as shown in Figure S3a-b. Moreover, as to the interface with multilayer As insertion, additional barrier at As region is introduced. In addition, the variations of the charge densities at interface regions are similar to those of Sc-mMoS_2 interfaces with BN and graphene insertions. These characters further confirm the results that we have concluded. To further confirm the results, the effective potentials rather than electrostatic potentials have been studied, as exhibited in Figure S3f-h. The tunneling barriers can be obtained from the effective potentials, and are marked in Figure S3f-h. The height and width of tunneling barriers can be used to evaluate the electron injection efficiency at interface region. It can be found from Figure 3f-h that additional tunneling barriers are introduced into Au-mMoS_2 interfaces with As insertions. Consequently, the enlarging total tunneling barriers enlarge and reducing electron injection efficiency with the increasing thickness of As insertions. These characters are consistent with Sc-mMoS_2 interfaces with BN and graphene insertions.