Interface Engineering of Au (111) for the Growth of 1T'-$MoSe_2$

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1. STM images of Se-pretreated Au(111)

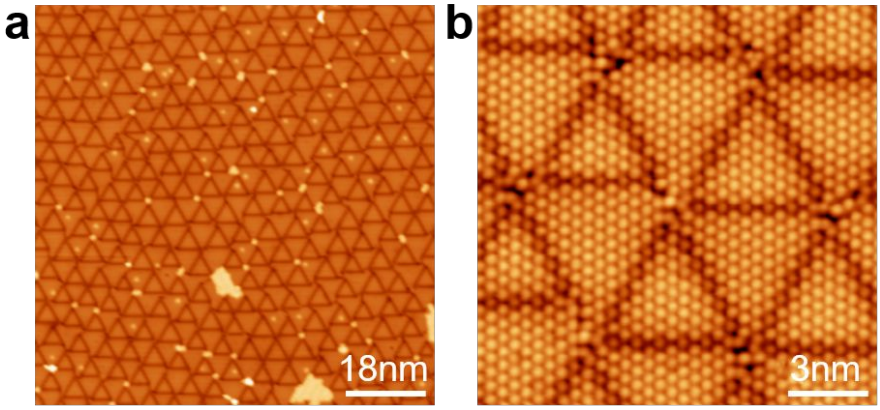

Figure S1. STM images of Se-pretreated Au(111). (a-b) Large-scale (a) and atomic-resolution (b) STM images of the Se-pretreated Au(111) substrate, showing the formation of $(\sqrt{3} \times \sqrt{3})$ R30°-Se/Au reconstruction.

2. DFT calculations of $MoSe_2$ with different phases on Au(111) and Mo-coated Au(111)

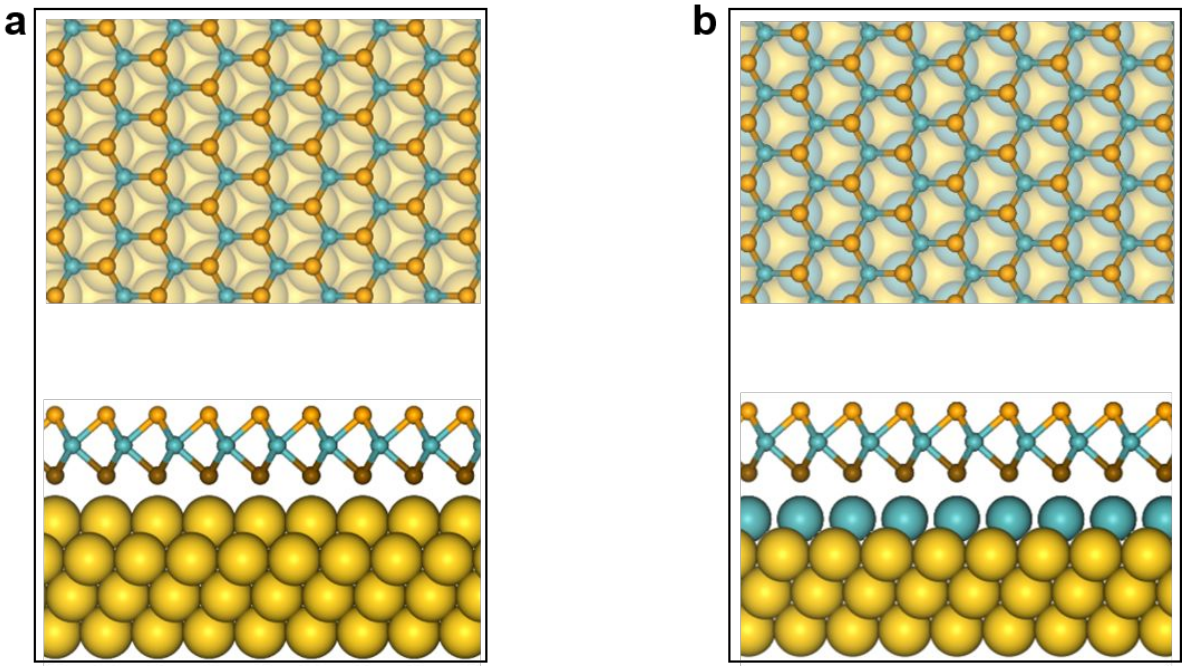

Figure S2. DFT calculations of 1H-$MoSe_2$ on Au(111) and Mo-coated Au(111). Atomic structures of 1H-$MoSe_2$ adsorbed on Au(111) (a) and Mo-coated Au(111) (b) in top (upper panel) and side (lower panel) views. The structure of $MoSe_2$ is indicated by ball-stick models, in which the orange, brown and blue balls represent Se atoms at the top sublayer, Se atoms at the bottom sublayer and Mo atoms respectively. Big spheres indicate the substrate atoms, in which golden and blue spheres represent Au and Mo atoms.

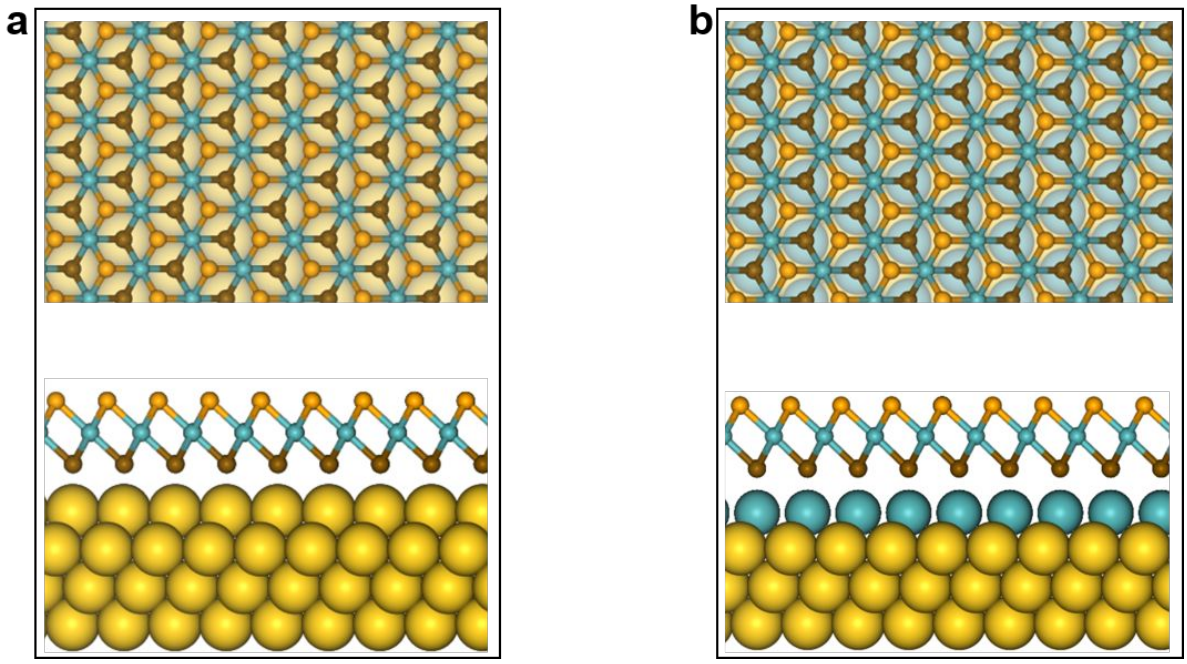

Figure S3. DFT calculations of 1T-$MoSe_2$ on Au(111) and Mo-coated Au(111). Atomic structures of 1T-$MoSe_2$ adsorbed on Au(111) (a) and Mo-coated Au(111) (b). Colour definition for atoms is the same as that in Figure S2.

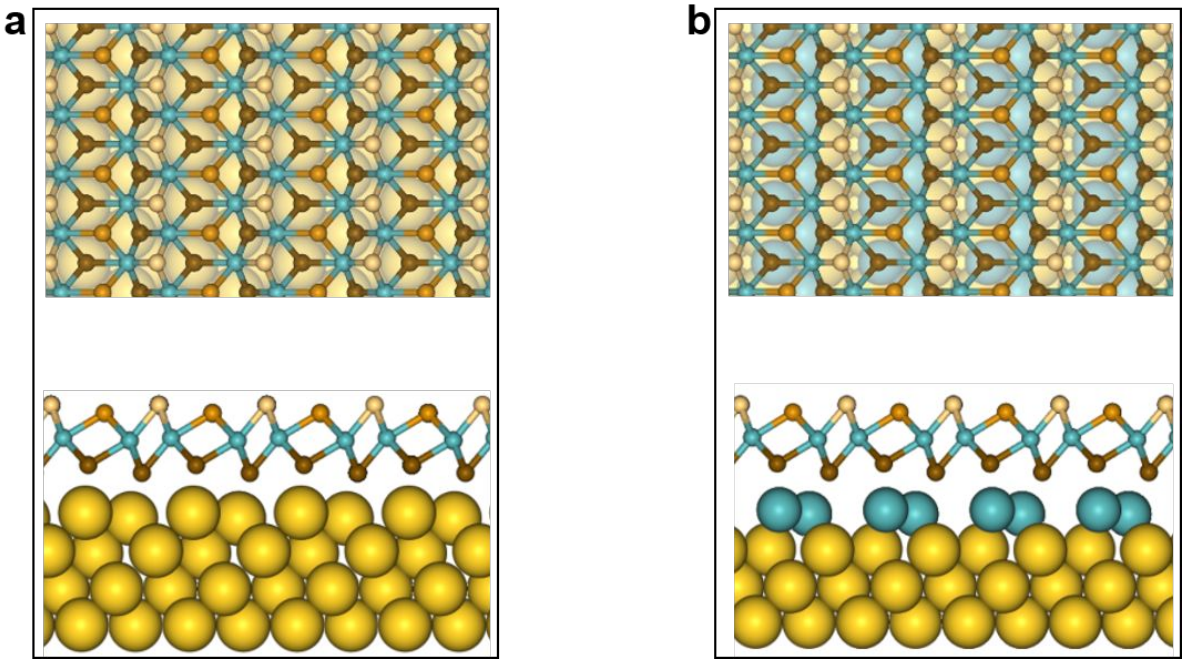

Figure S4. DFT calculations of 1T'-$MoSe_2$ on Au(111) and Mo-coated Au(111). Atomic structures of 1T'-$MoSe_2$ adsorbed on Au(111) (a) and Mo-coated Au(111) (b). Colour definition for atoms is the same as that in Figure S2. In addition, Se atoms at the top sublayer are distinguished by two colours for different heights.

3. Partial density of states calculations.

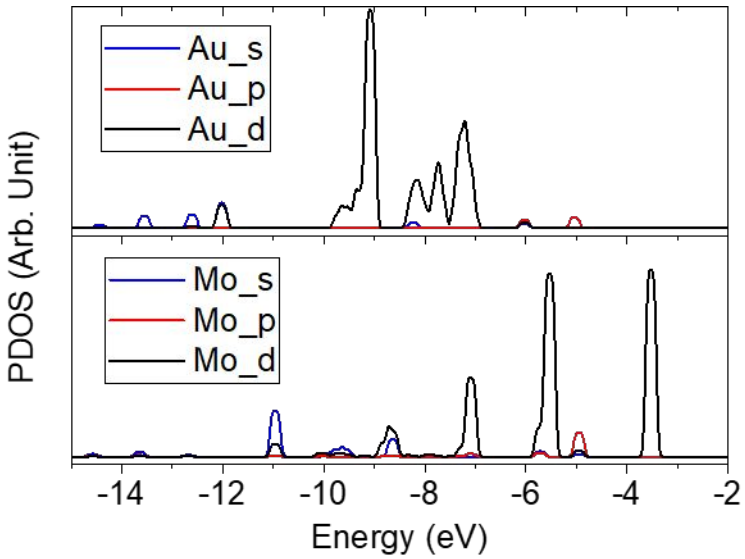

Figure S5. Calculated partial density of states for the surface atom on Au(111) substrate (top) and Mo-coated Au(111) substrate (bottom). States for s, p and d orbitals are separated. The vacuum energy is set as the zero point.