

Barrier-Free Carrier Injection in 2D WSe₂/MoSe₂

Heterostructures via Fermi-Level Depinning

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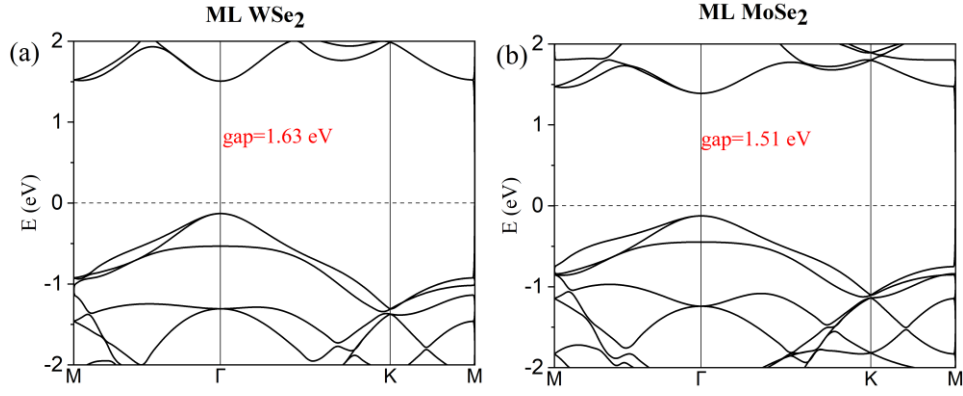


Fig. S1. Band structures of (a) pure ML WSe₂($\sqrt{3}\times\sqrt{3}$) and (b) ML MoSe₂($\sqrt{3}\times\sqrt{3}$), exhibiting a direct band gap of 1.63 eV and 1.51eV, respectively.

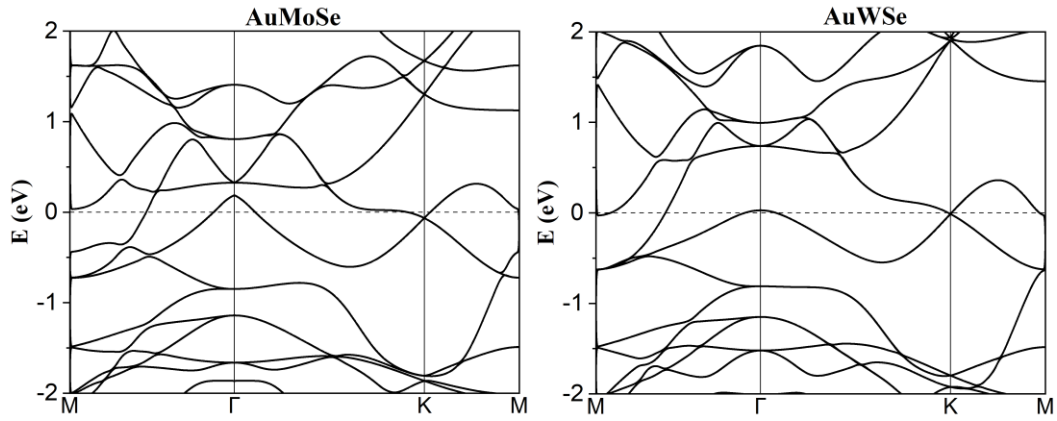


Fig. S2. Band structures of Au-doped MoSe₂ and WSe₂, the zero-bandgap metallic characteristics were obtained.

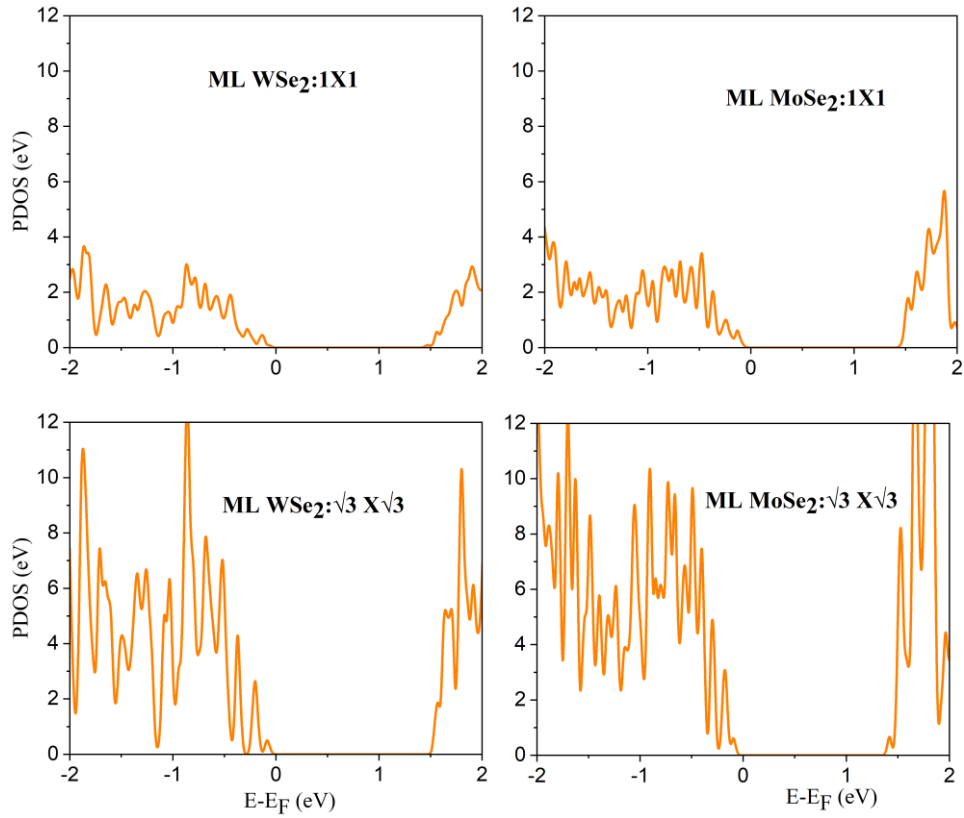


Fig. S3. Partial density of states (PDOS) for pristine ML WSe₂ and MoSe₂. The Fermi level is set at zero.

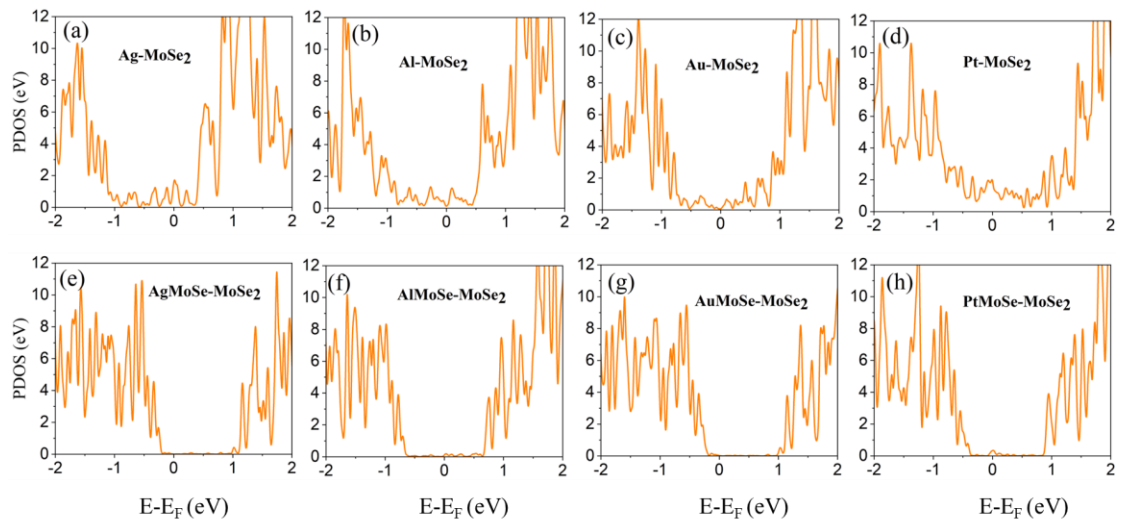


Fig. S4. Partial density of states (PDOS) of MoSe₂ after contact with (a)-(d) metals and (e)-(h) metallic mMoSe surfaces. The Fermi level is at zero energy.

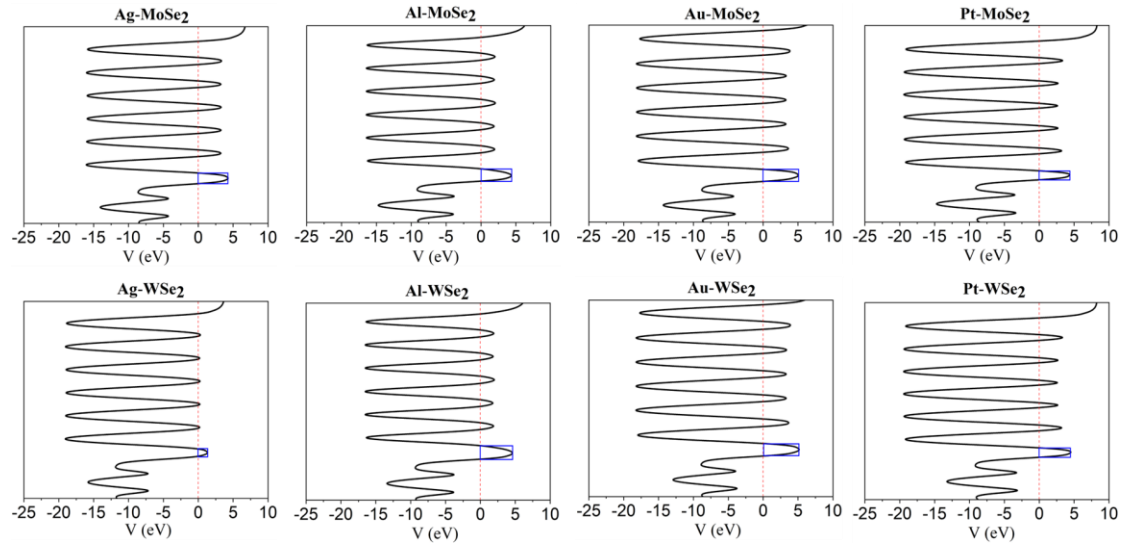


Fig. S5. Average electrostatic potential V in planes normal to ML metal-WSe₂/MoSe₂ contacts. The Fermi level is zero, as indicated by the red dash lines.