

## Supporting Information

### Interfacial electronic properties between PtSe<sub>2</sub> and 2D metal electrodes: a first-principles simulation

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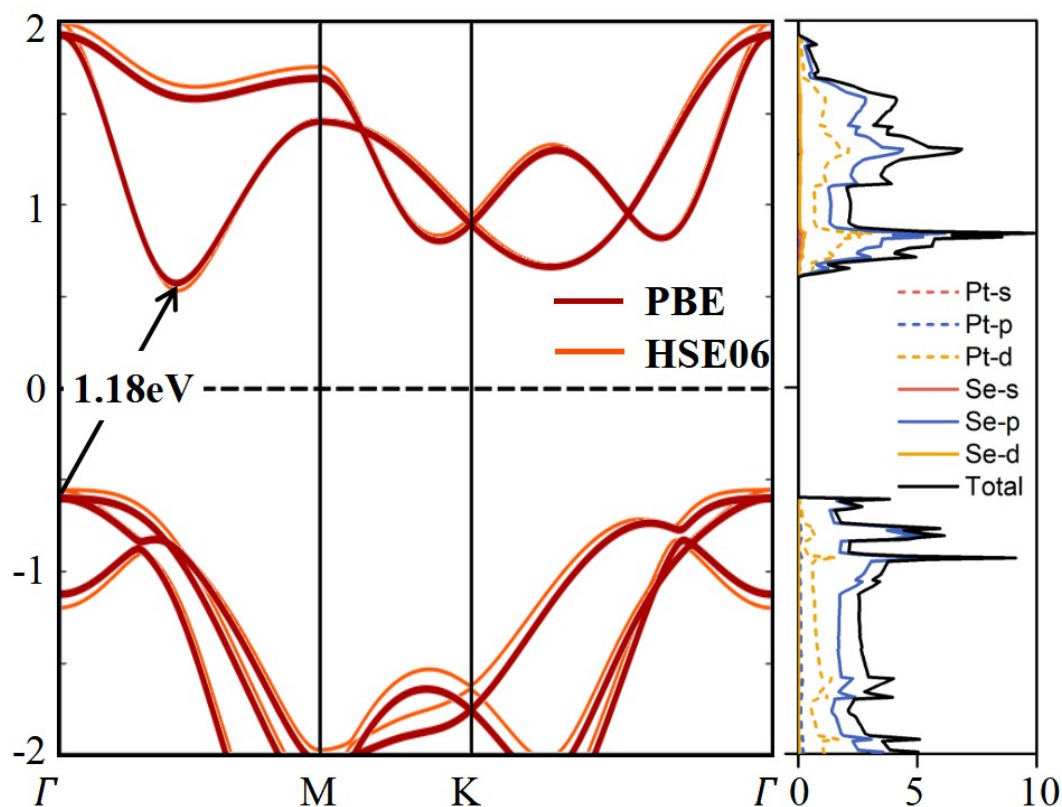


Figure S1. Band structure and PDOS of PtSe<sub>2</sub>. The Fermi level is set to zero energy and represented by the black dashed line.

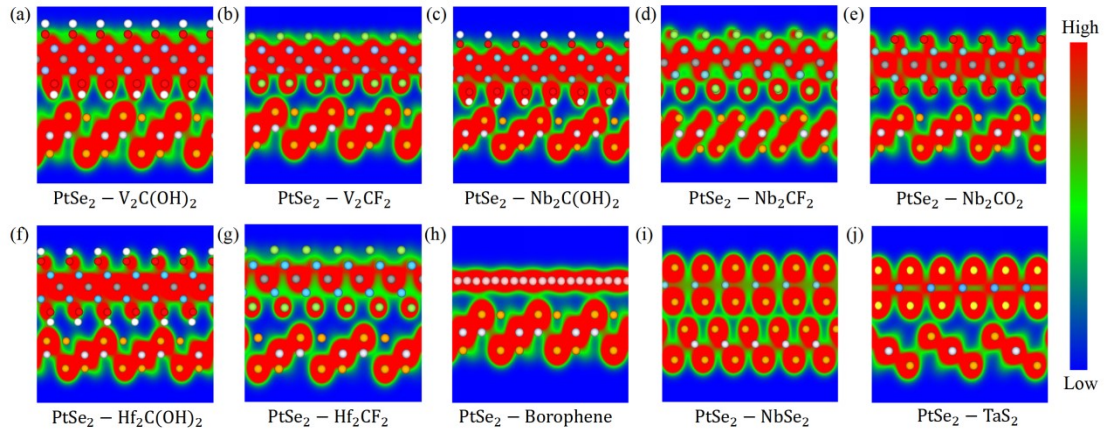


Figure S2. Electron localization function of the  $PtSe_2$ -2D metal.

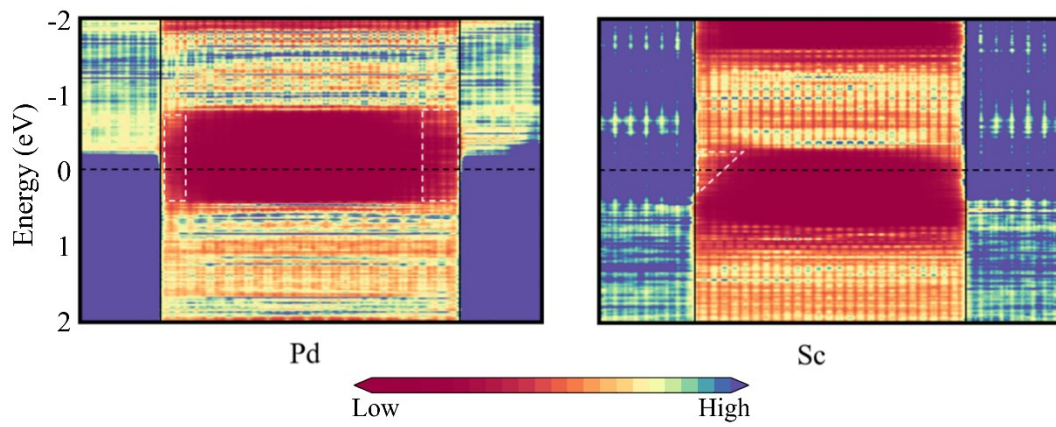


Figure S3. LDDOS of Pd/Sc-PtSe<sub>2</sub> FETs at zero bias voltage. The black dashed line is the Fermi energy level, the white dash box is the MIGs.