

Supplementary Information

Inversion Domain Boundaries in MoSe₂ Layers

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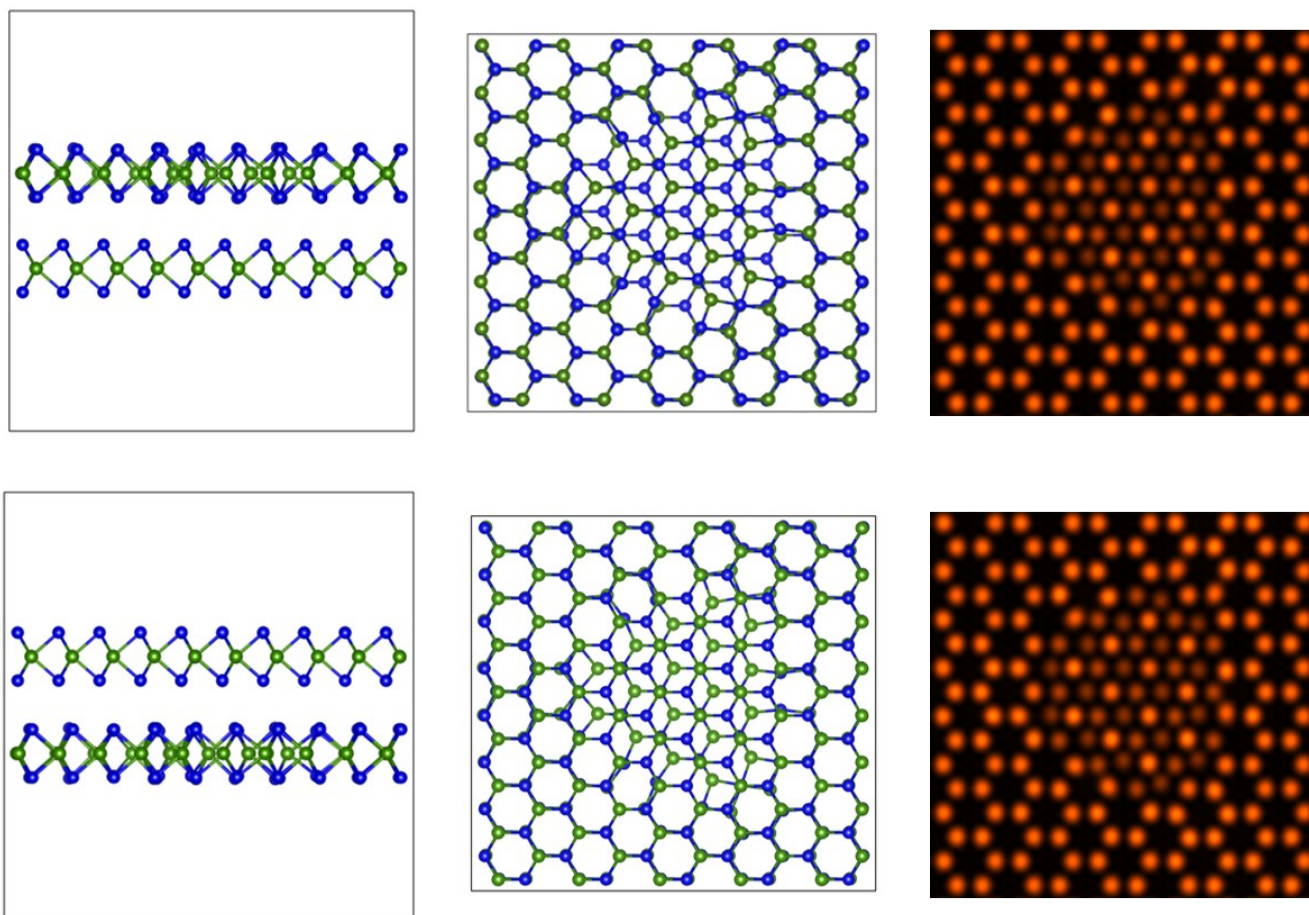


Fig. S1 Change in layer stacking sequence (left) does not change the simulated HAADF image (right).
 (Top) The defect layer on top of perfect layer. (Bottom) The perfect layer on top of defect layer.

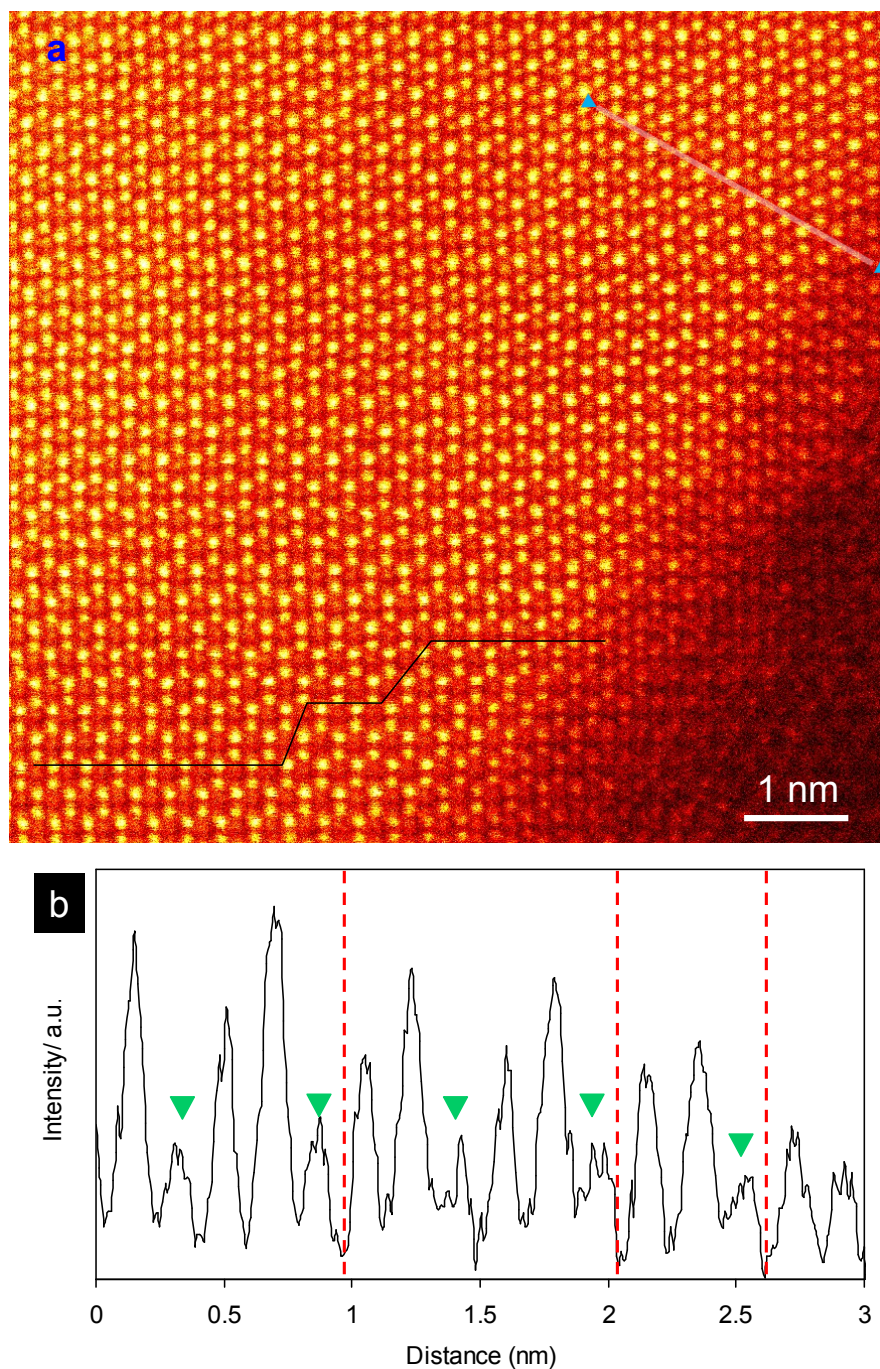


Fig. S2 Inversion domains boundary in MoS₂. (a) HAADF image of MoS₂ nanosheets. The dark line indicate the stacking boundaries of 2H and 3R phase. (b) Image intensity profile acquired along the white line in (a). The red dashed lines indicate layer step position. The green triangles indicate the position of visible contrast in the center of hexagonal rings.

Estimation of formation energy. The formation energy per unit length is defined as $\Delta E_{\text{Form}} = (E_{\text{System}} - N_{\text{Mo}} \times E_{\text{Mo_ML}} - N_{\text{Se}} \times E_{\text{Se_ML}})/L$, where N_{Mo} and N_{Se} are, respectively, the number of Mo and Se atoms in the system, L is total length of the IDBs in the system, and $E_{\text{Mo_ML}} = E_{\text{Mo}} + E_{\text{Bond}}$ and $E_{\text{Se_ML}} = E_{\text{Se}} + E_{\text{Bond}}$ are energies of Mo and Se atoms in a monolayer without IDBs, in which $E_{\text{Bond}} = (E_{\text{ML}} - E_{\text{Mo}} - 2E_{\text{Se}})/3$, where E_{ML} , E_{Mo} , and E_{Se} are the energies of the monolayer MoSe_2 and Mo and Se atoms in bulk, respectively. In Fig. S3, we show the 8-fold and 4-fold rings in the hexagonal lattice of the monolayer MoSe_2 , which are used to calculate the formation energy.

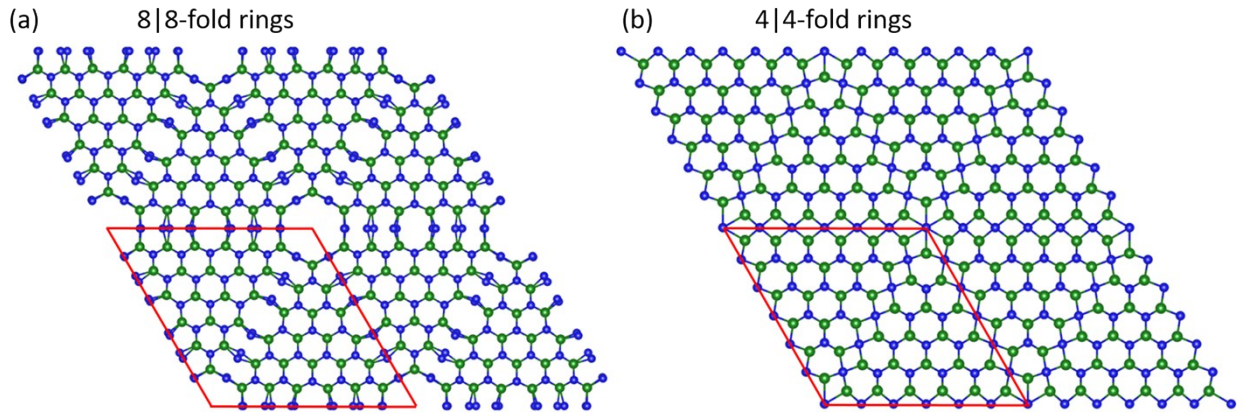


Fig. S3 Construction of the structures of (a) 8- and (b) 4-fold boundaries in the hexagonal lattice of the monolayer MoSe_2 . The solid black box represents the supercell.