### **Supplementary Information to**

# Nanoscale island manipulation and construction of heterojunction by mechanical collision of 2D materials

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### 1. STM images of H-NbSe<sub>2</sub> islands on BLG/SiC

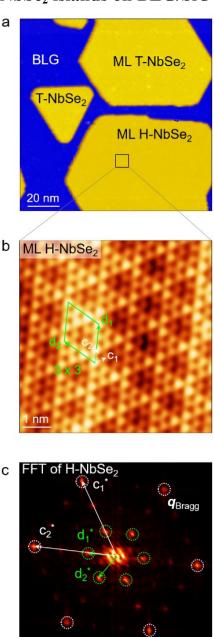


Figure S1: Atomic-resolution STM images of monolayer H-NbSe<sub>2</sub> islands. (a) STM image of monolayer H-phase and T-phase NbSe<sub>2</sub> islands epitaxially grown on a bilayer graphene (BLG)/SiC(0001) substrate. (b) Zoom-in STM image of the region marked by the black square in (a), revealing the typical <sup>3</sup> × <sup>3</sup> charge density wave (CDW) pattern and the atomic-resolution structure of monolayer H-NbSe<sub>2</sub>. (c) FFT image corresponding to (b), highlighting the periodic CDW modulation and the underlying atomic lattice of the H-phase.

### 2. Coexistence of T- and H-phase on one NbSe2 island

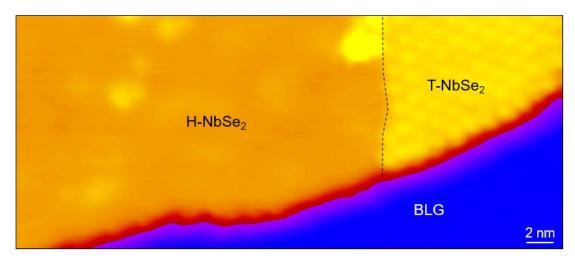


Figure S2: STM image of coexistence of T- and H-phase on one NbSe<sub>2</sub> island.

## 3. STM tip manipulation to cause translation of T-NbSe<sub>2</sub> islands laterally and collide with H-NbSe<sub>2</sub>

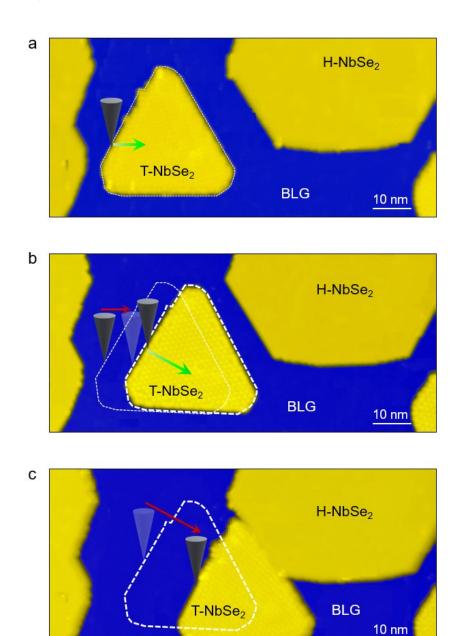


Figure S3: Translation of T-NbSe2 islands laterally and collision with H-NbSe2.

(a) Initial configuration of T-phase NbSe<sub>2</sub> and H-phase NbSe<sub>2</sub> islands before STM tip manipulation. The green arrow indicates the starting position of the STM tip and its movement trajectory during manipulation. (b) STM topographic image after the first tip manipulation. The white dashed box marks the original position of the T-phase NbSe<sub>2</sub> island. The green arrow shows the lateral movement path of the tip during the

second translational manipulation. (c) STM image following the second translational manipulation. A collision between the T-phase NbSe<sub>2</sub> and H-phase NbSe<sub>2</sub> islands is observed, but no structural and phase transition is detected. These results demonstrate that, in contrast to rotational manipulation, the translational displacement cannot induce a phase transition in the NbSe<sub>2</sub> system.

## 4. Atomic-resolution STM images at the edge of monolayer $T\text{-NbSe}_2$ and $H\text{-NbSe}_2$ islands

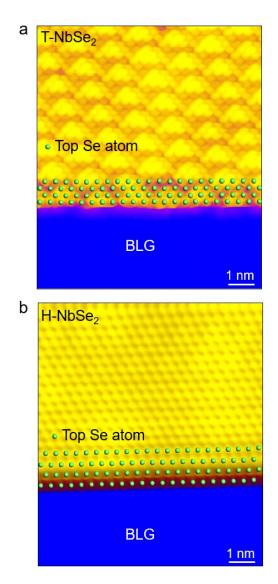
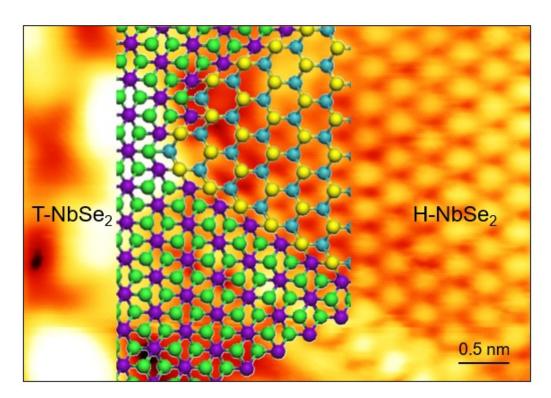


Figure S4. Atomic-resolution STM images at the edge of monolayer (a) T-NbSe<sub>2</sub> and (b) H-NbSe<sub>2</sub> islands. The atomic structures of the top Se atoms are superposed on the image, demonstrating that the edge of T- and H-NbSe<sub>2</sub> exhibits a well-ordered Se-terminated zigzag configuration.

### 5. Schematic model of the heterojunction



**Figure S5: Schematic model of the heterojunction after phase transition.** In T-NbSe<sub>2</sub>, the Nb and Se atoms are represented by the purple and green balls respectively. In H-NbSe<sub>2</sub>, the Nb and Se atoms are represented by the blue and yellow balls, respectively.