

Atomic-scale dynamics of the phase transition in bilayer PtSe₂

Lei Xu,^a Lifen Wang,^{b, c} Huan Liu,^a Feng Li,^d Delong Li,^d Yongwan Cao,^a ChenChen Wu,^a Xuedong Bai,^{*b, c, e} and Junjie Qi^{*a}

^a *School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, People's Republic of China.*

^b *Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

^c *Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China*

^d *Collaborative Innovation Centre for Optoelectronic Science & Technology, and Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, Institute of Microscale Optoelectronics, College of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen, Guangdong 518060, China.*

^e *School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China*

*Corresponding author email address:

junjieqi@ustb.edu.cn, xdbai@iphy.ac.cn

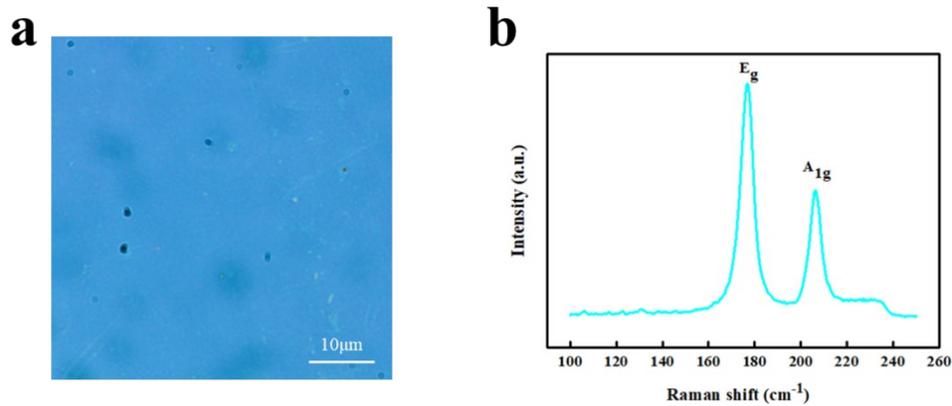


Figure S1 (a) Optical microscope image of PtSe₂ on a SiO₂/Si substrate, (b) Raman spectra of PtSe₂.

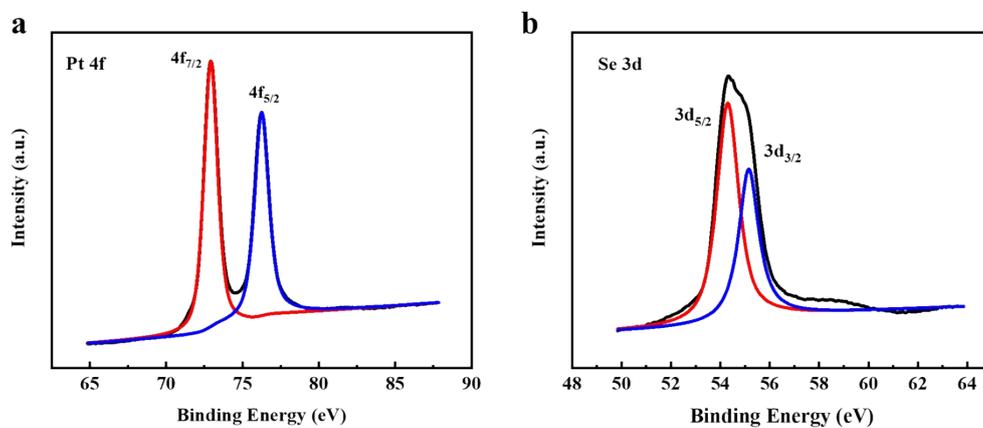


Figure S2 High-resolution XPS spectra of (a) Pt 4f and (b) 3d.

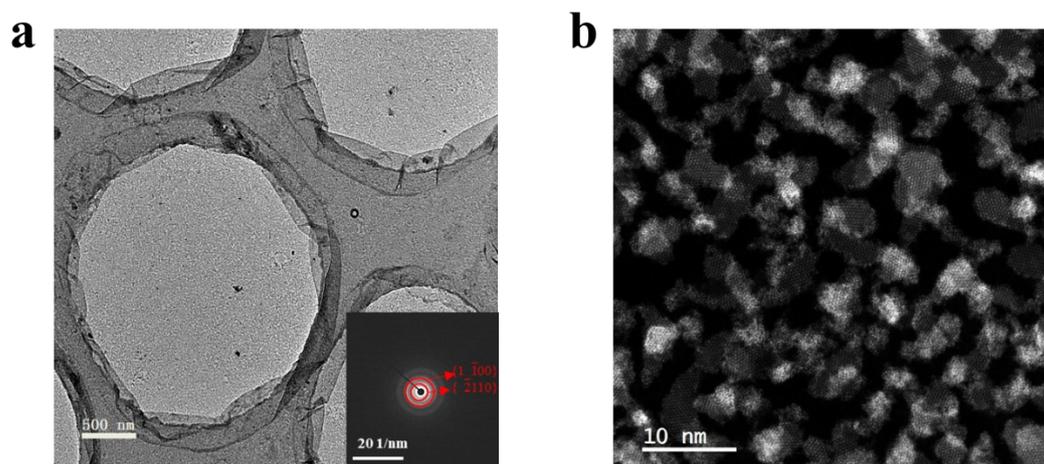


Figure S3 (a) Low magnification TEM image, the inset is the selected area diffraction pattern of the PtSe₂ film. (b) STEM-ADF image of PtSe₂ film.

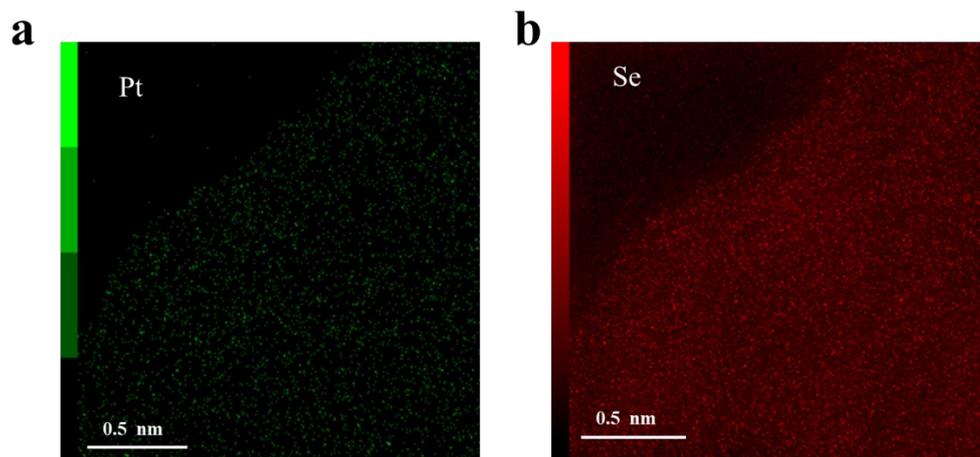


Figure S4 (a) EDS element mappings of Pt and (b) EDS element mappings of Se.

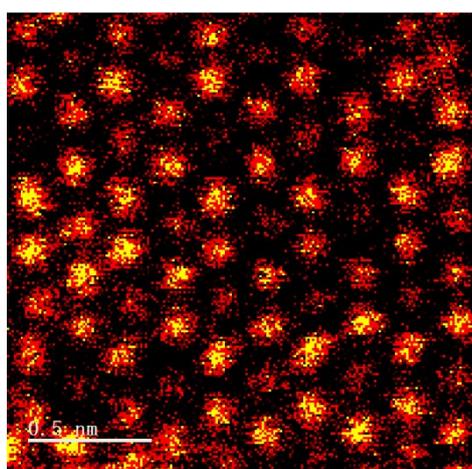


Figure S5 Atomic-resolution STEM-ADF images of the 3R phase of bilayer PtSe₂.

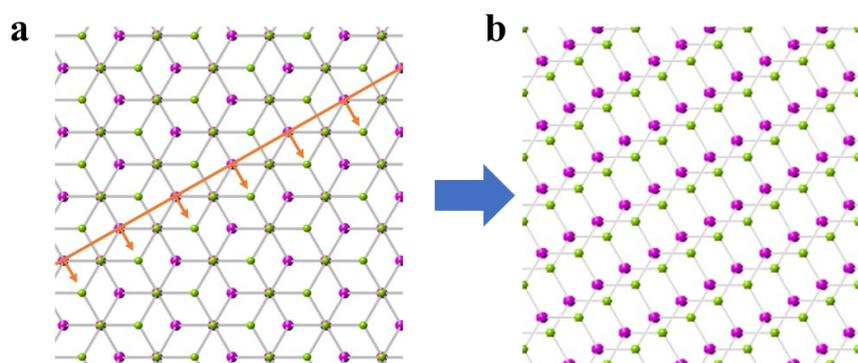


Figure S6 (a) Schematic for AB stacked bilayer PtSe₂. Orange arrows indicate the direction of the interlayer shift. (b) Schematic for shifted bilayer PtSe₂ based on a. Pt, pink; Se, green.

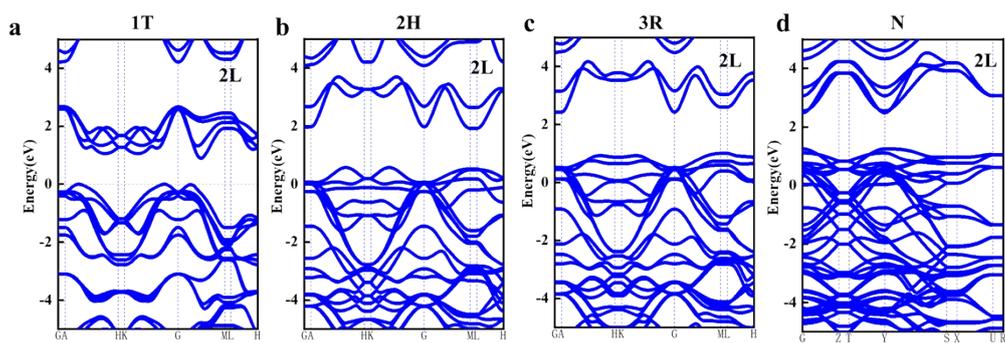


Figure S7 Band structures of 1T(a), 2H(b), 3R(c) and N (d) phase of bilayer PtSe₂.

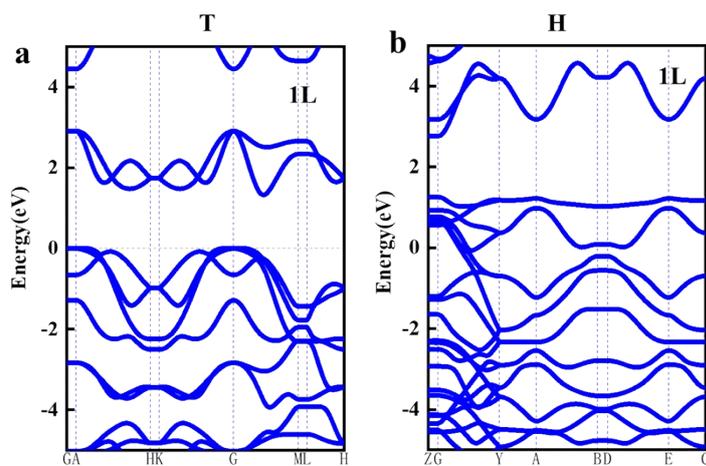


Figure S8 Band structures of T (a) and H (b) phase of monolayer PtSe₂.

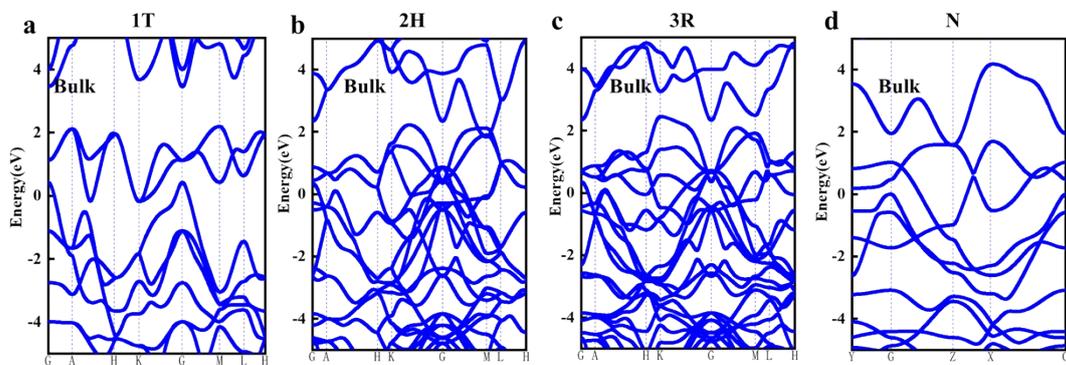


Figure S9 Band structures of 1T(a), 2H(b), 3R(c) and N (d) phase of bulk PtSe₂.

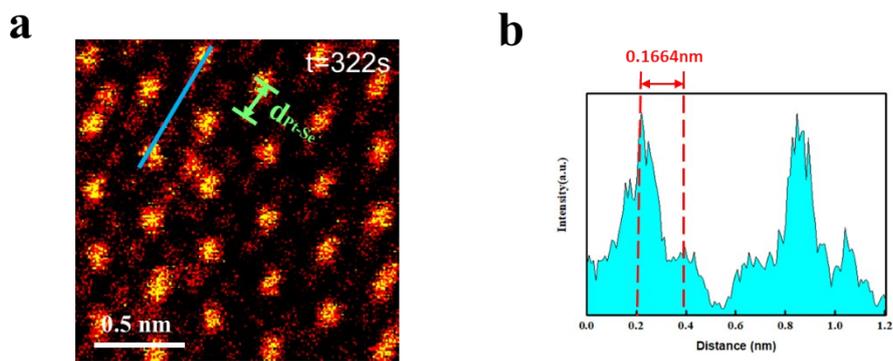


Figure S10 (a) ADF image in Figure 3a; (b) The intensity line profiles from the blue line.

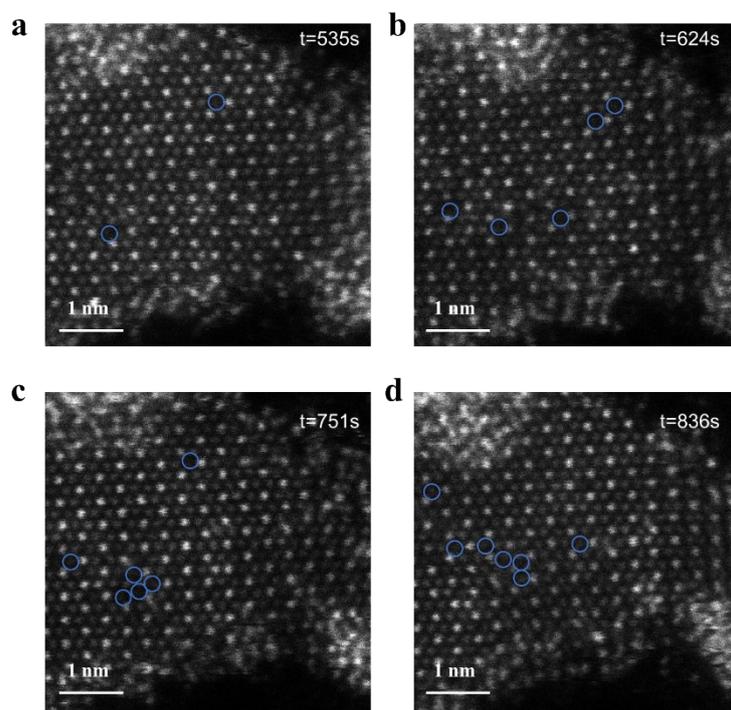


Figure S11 1T phase of PtSe_2 (1T was obtained from 2H phase transition.) under the electron beam irradiation. Under the electron beam irradiation, the thermodynamically stable 1T phase structure of PtSe_2 did not changed. Blue circles in Figure S11 indicate the location of the Se vacancies in the film.