Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION

The structural superlubricity at the interface of penta-BN_2

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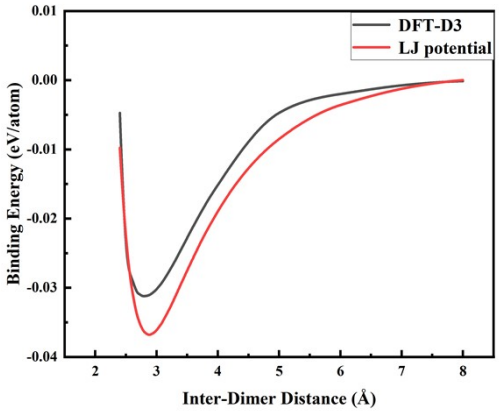

Fig.S1 Binding energy of the bilayer penta-BN_2 calculated by the many-body dispersion effects corrected density functional theory (DFT-D3) method and Lennard-Jones (LJ) potential.

Fig.S2 Diagram showing the sliding directions on the surface of penta-BN_2 monolayer.

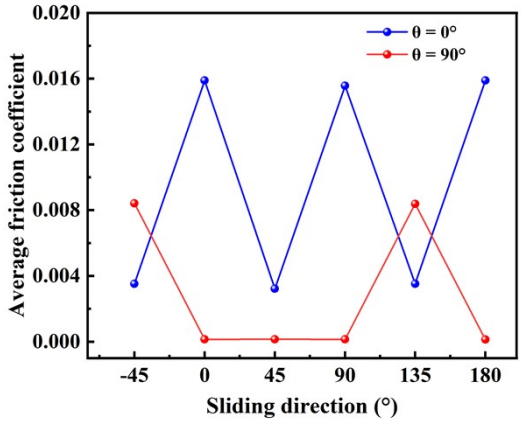

Fig.S3 The averaged friction coefficients along -45°, 0°, 45°, 90°, 135° and 180° sliding direction at the interface of the bilayer penta-BN_2 with twist angles of 0° and 90°.

Fig.S4 A snapshot for the sliding along the direction of 135°at the interface of bilayer penta-BN_2 with the twist angle of 90°.

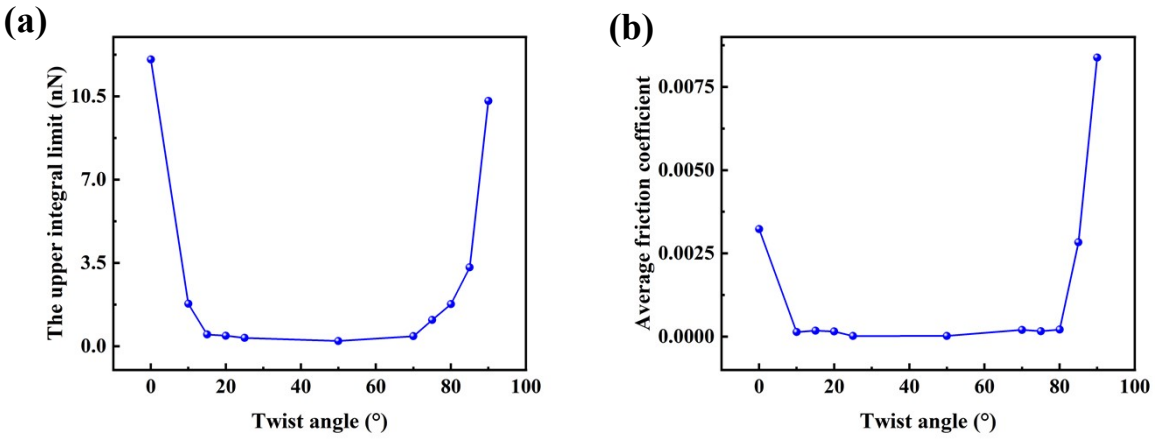

Fig.S5 (a) The upper limit of the integral along 135° sliding direction at the interface of the relatively rotated bilayer penta-BN_2 with quasi-harmonic periodic oscillation. (b) The averaged friction coefficient along 135° sliding direction at the interface of the relatively rotated bilayer penta-BN_2 with quasi-harmonic periodic oscillation.

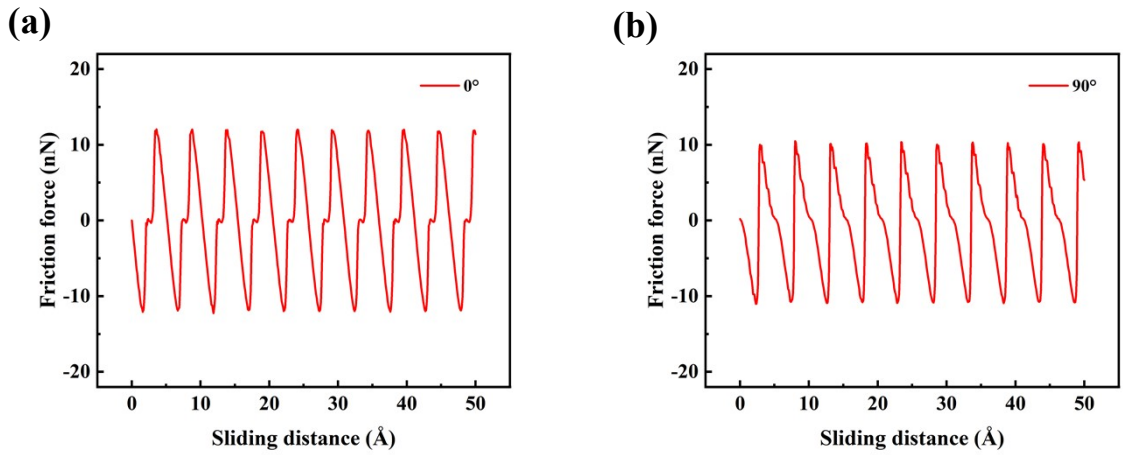

Fig.S6 The friction force along 135° sliding direction at the interface of the relatively rotated bilayer penta-BN_2 with twist angles of (a) 0° and (b) 90°.

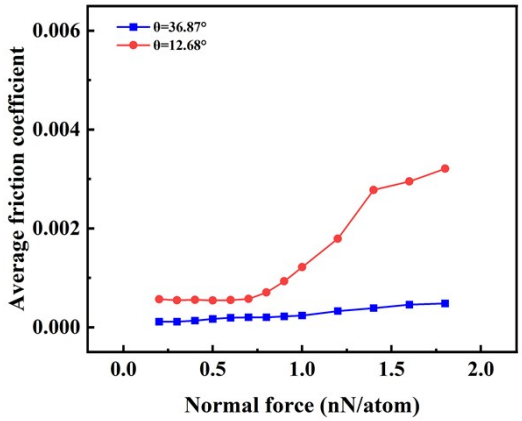

Fig.S7 The evolution of the averaged friction coefficient at the interface of relatively rotated bilayer penta-BN_2 with twist angles of 36.87° and 12.68° with respect to the normal force of 0.2 ~ 1.8 nN/atom via adopting the larger size (1260 atoms) slider.

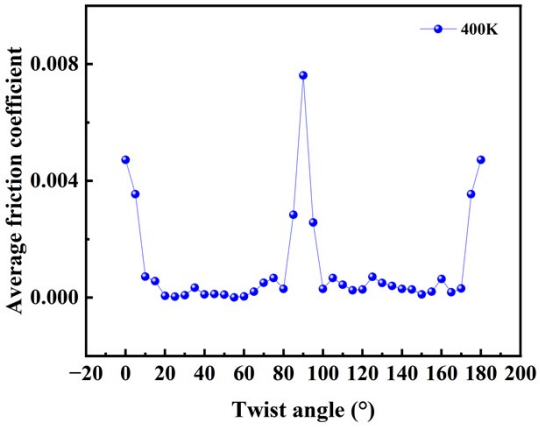

Fig.S8 The averaged friction coefficients along 135° sliding direction at the interface of the relatively rotated bilayer penta-BN_2 with twist angles of 0° ~ 180° at 400K.