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

Supplementary Materials

Physisorption energy data for Neon – BN surfaces

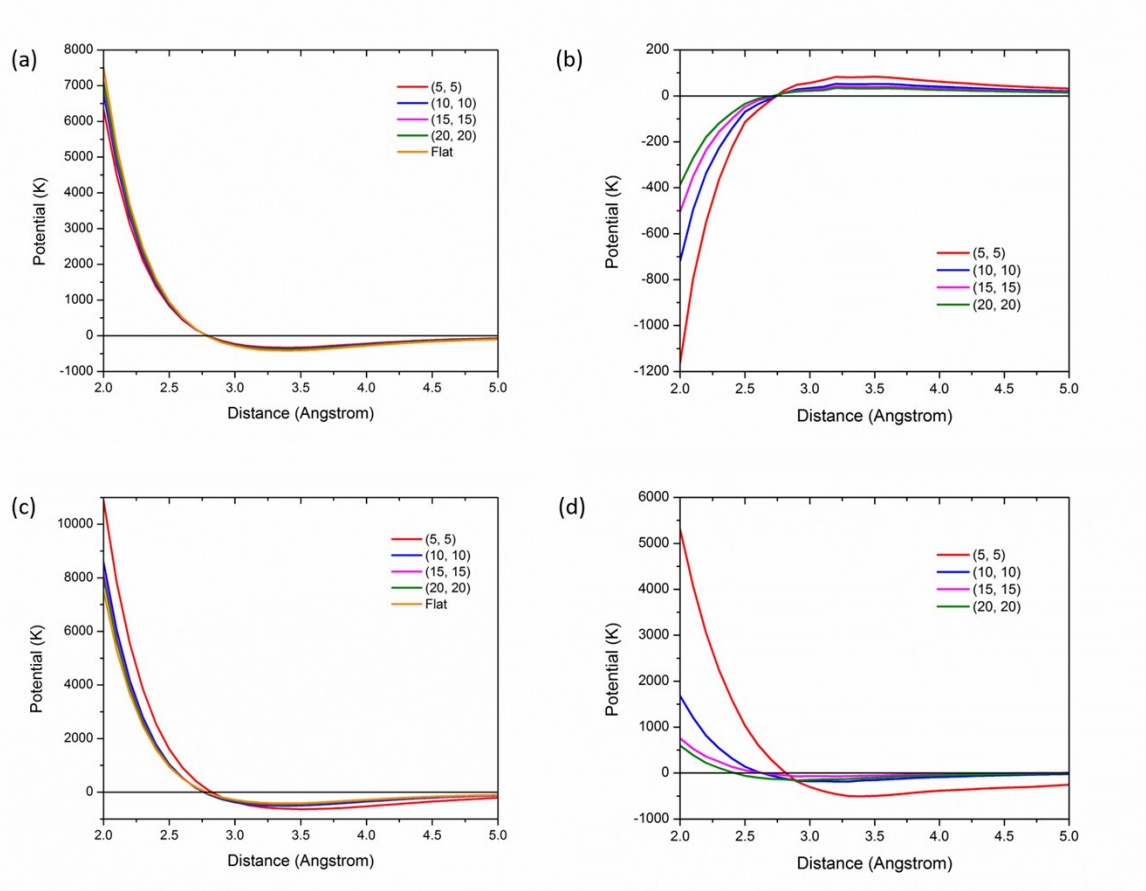

Figure S1. Ne – BN surfaces (a) convex side potential energy; (b) convex side potential energy difference; (c) concave side potential energy; (d) concave side potential

Physisorption energy data for H_2O – BN surfaces

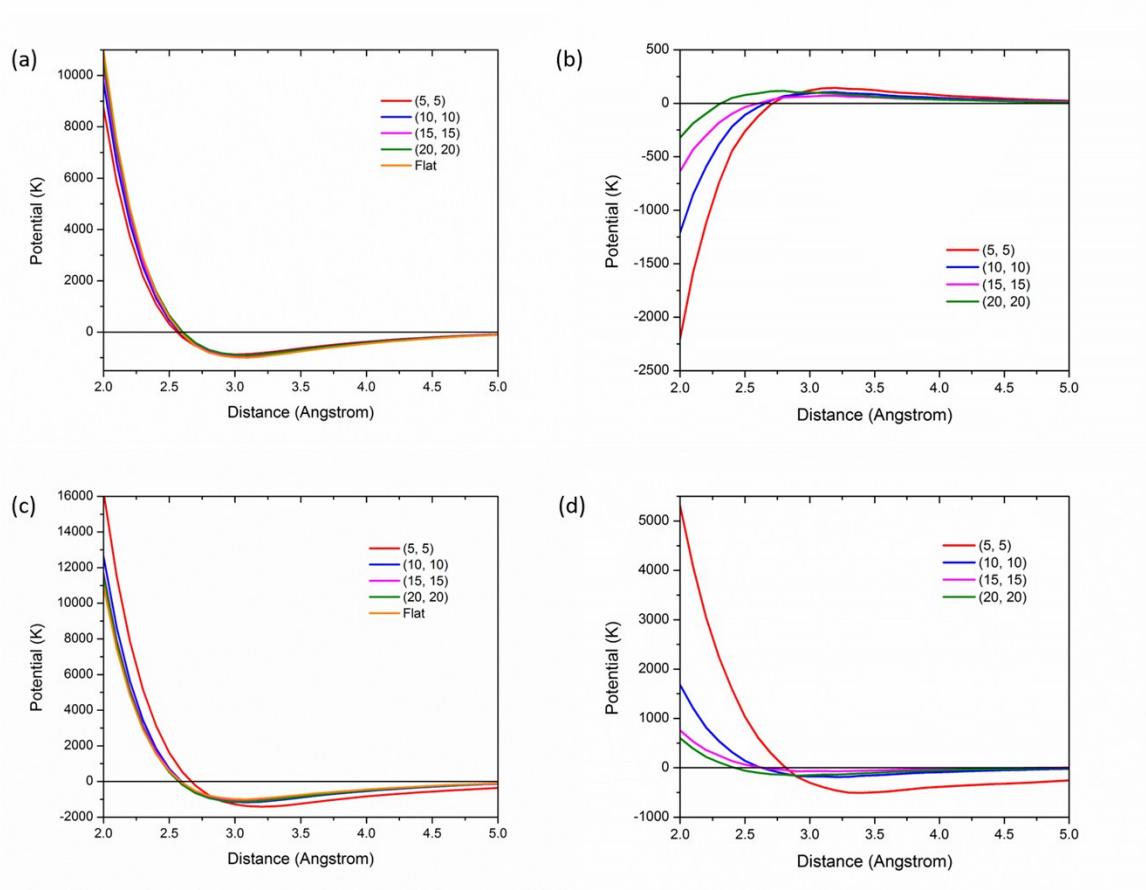

Figure S2. H_2O – BN surfaces (a) convex side potential energy; (b) convex side potential energy difference; (c) concave side potential energy; (d) concave side potential. The H_2O molecule is oriented perpendicularly to the BN surface with the oxygen atom near and hydrogen atoms away from the surface.

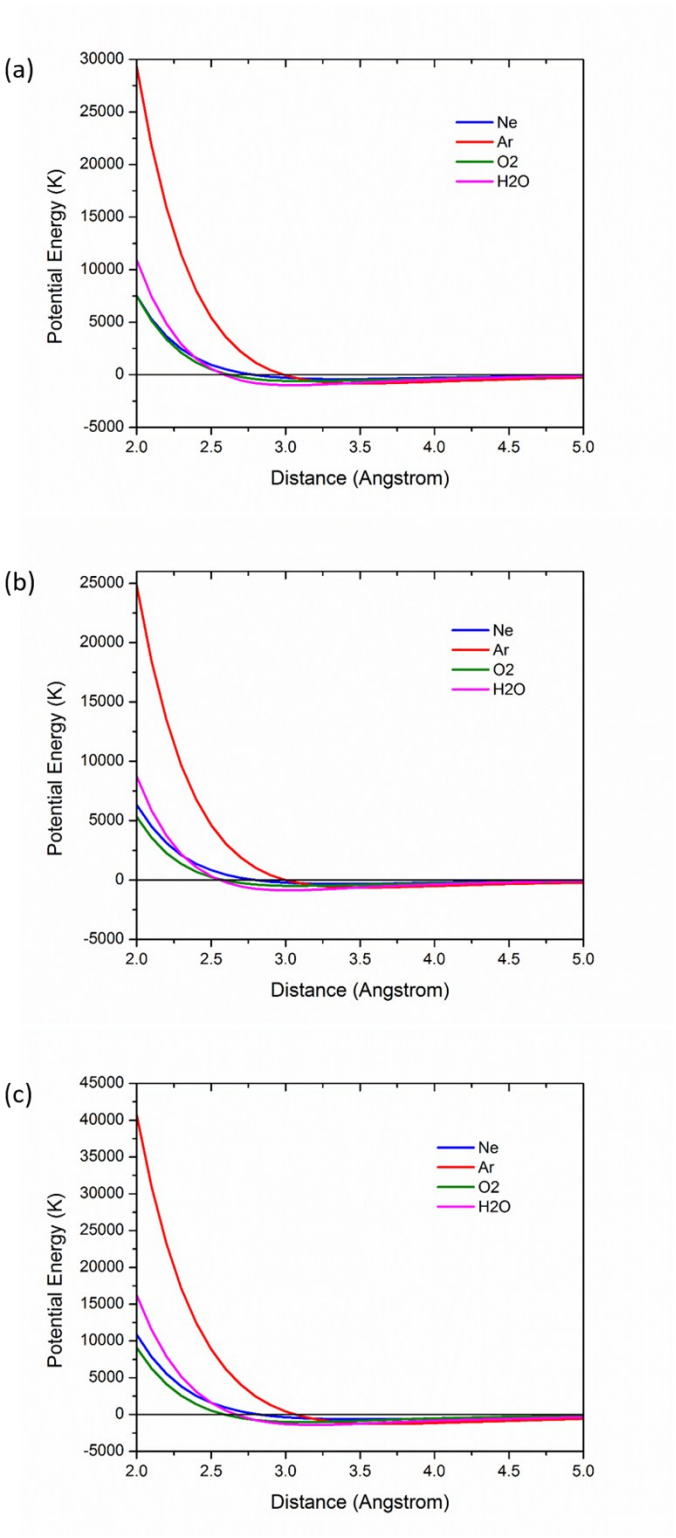

Figure S3. Potential energy comparison between adsorbents: (a) flat BN surface, (b) (5, 5) surface convex side, (c) (5, 5) surface concave side.

HOMO, LUMO orbitals plots:

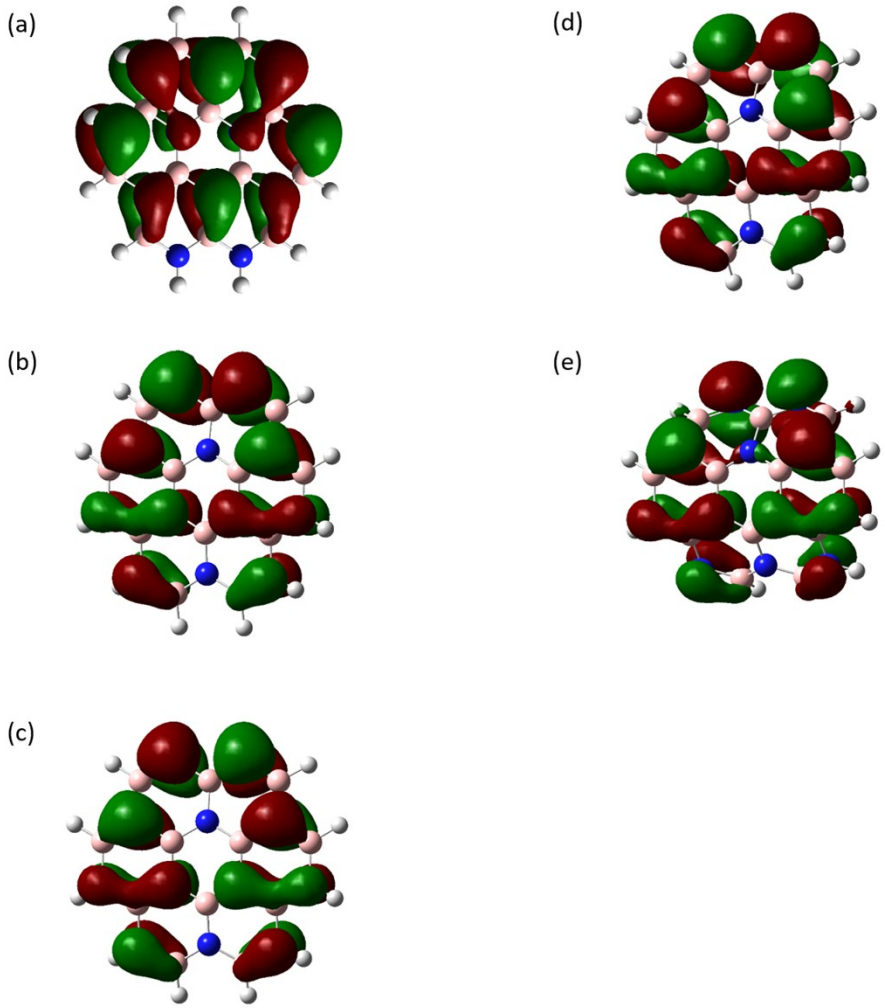

Figure S4. HOMO orbitals of the BN surfaces: (a) (5,5), (b) (10,10), (c) (15,15), (d) (20,20), (e) flat

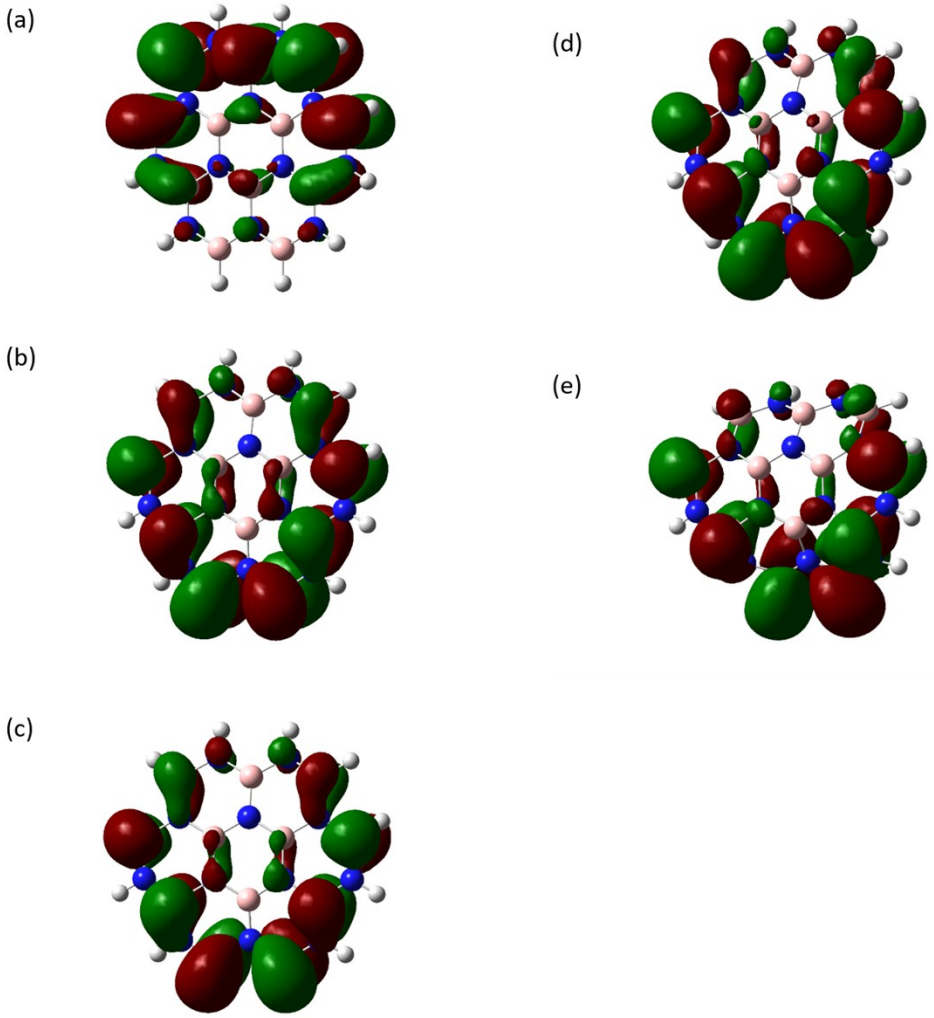

Figure S5. LUMO orbitals of the BN surfaces: (a) (5,5), (b) (10,10), (c) (15,15), (d) (20,20), (e) flat