

Supporting Information

Adsorption of the Atmospheric Gas Molecules (NH₃, H₂S, CO, H₂, CH₄, NO, NO₂, C₆H₆ and C₃H₆O) on Two-Dimensional Polyimide with Hydrogen Bonding: A First-principles Study

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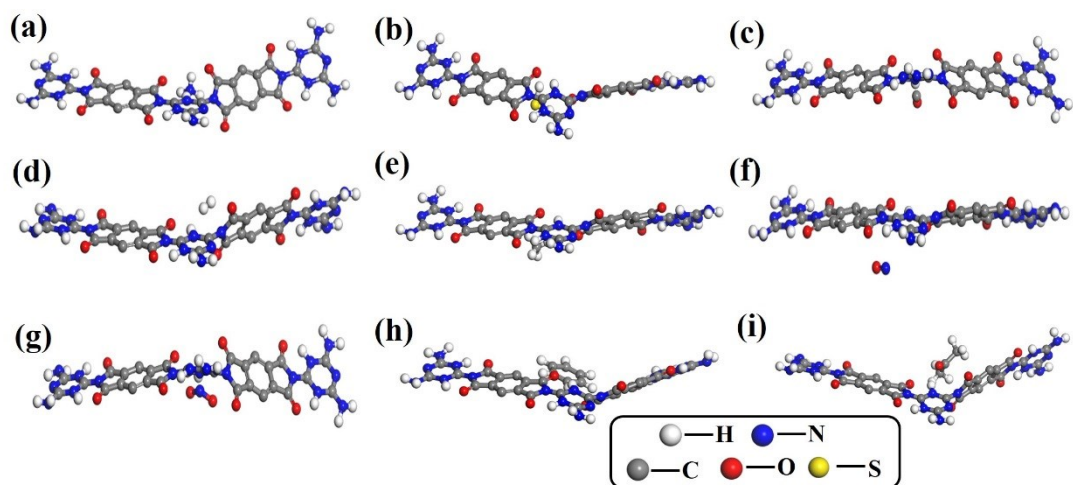


Figure S1. Side view of optimized geometric structures of (a) NH_3 , (b) H_2S , (c) CO , (d) H_2 , (e) CH_4 , (f) NO , (g) NO_2 , (h) C_6H_6 , (i) $\text{C}_3\text{H}_6\text{O}$ gas molecules adsorbed on position 1 of polyimide (1-2DPI).

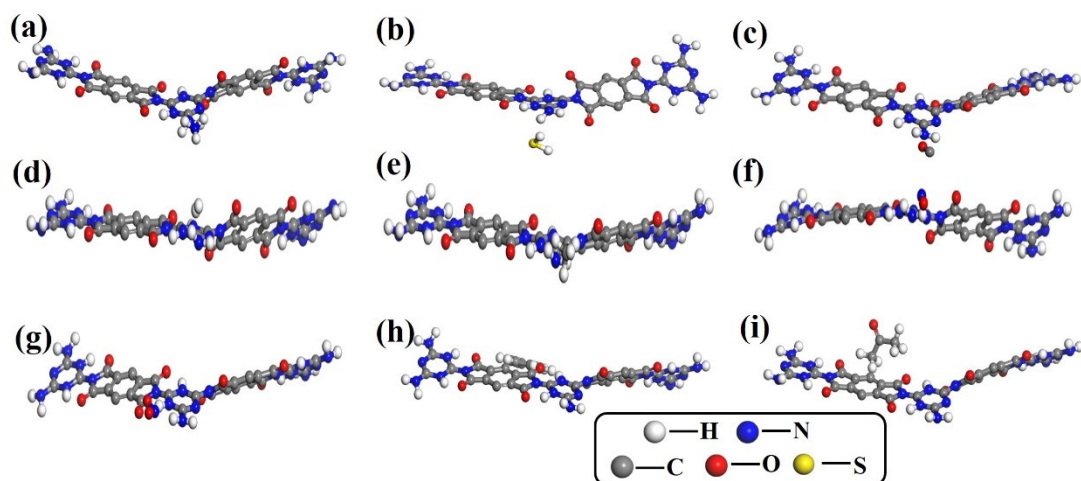


Figure S2. Side view of optimized geometric structures of (a) NH_3 , (b) H_2S , (c) CO , (d) H_2 , (e) CH_4 , (f) NO , (g) NO_2 , (h) C_6H_6 , (i) $\text{C}_3\text{H}_6\text{O}$ gas molecules adsorbed on position 2 of polyimide (2-2DPI).

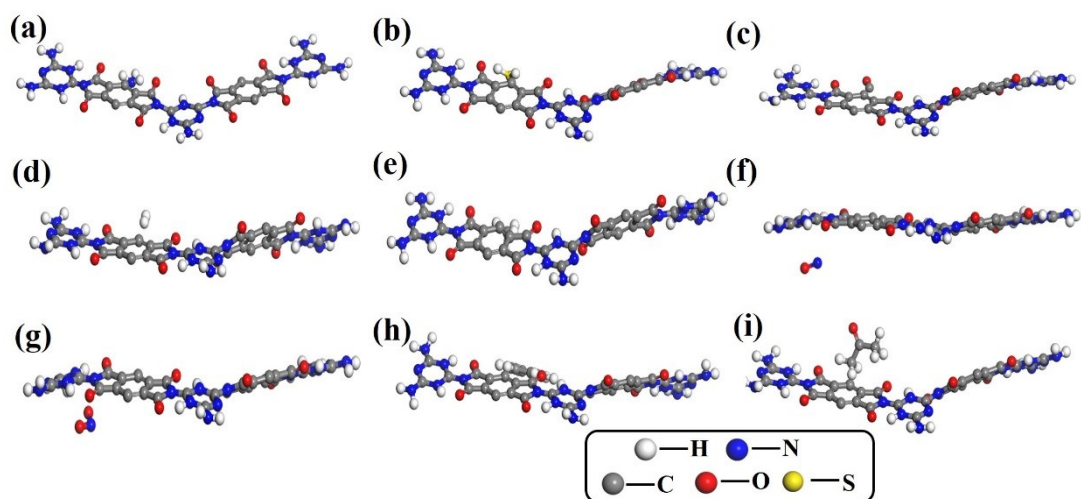


Figure S3. Side view of optimized geometric structures of (a) NH₃, (b) H₂S, (c) CO, (d) H₂, (e) CH₄, (f) NO, (g) NO₂, (h) C₆H₆, (i) C₃H₆O gas molecules adsorbed on position 3 of polyimide (3-2DPI).

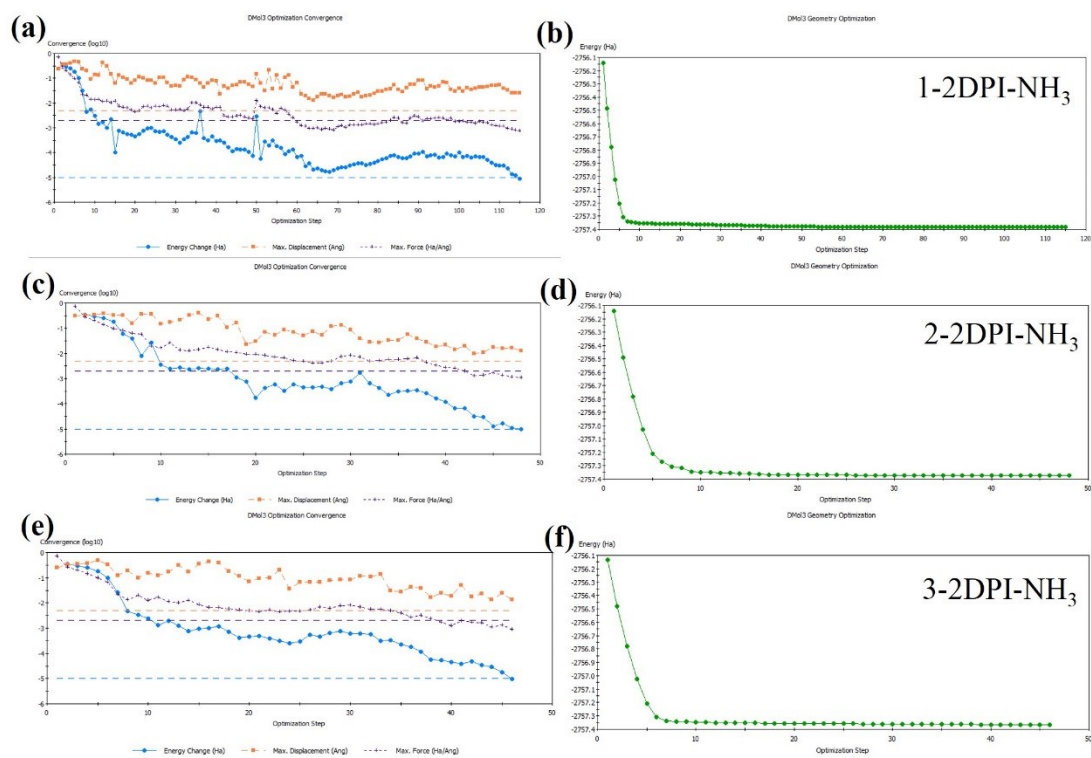


Figure S4. The relationship between convergence, energies and optimization step of NH₃ adsorption system.

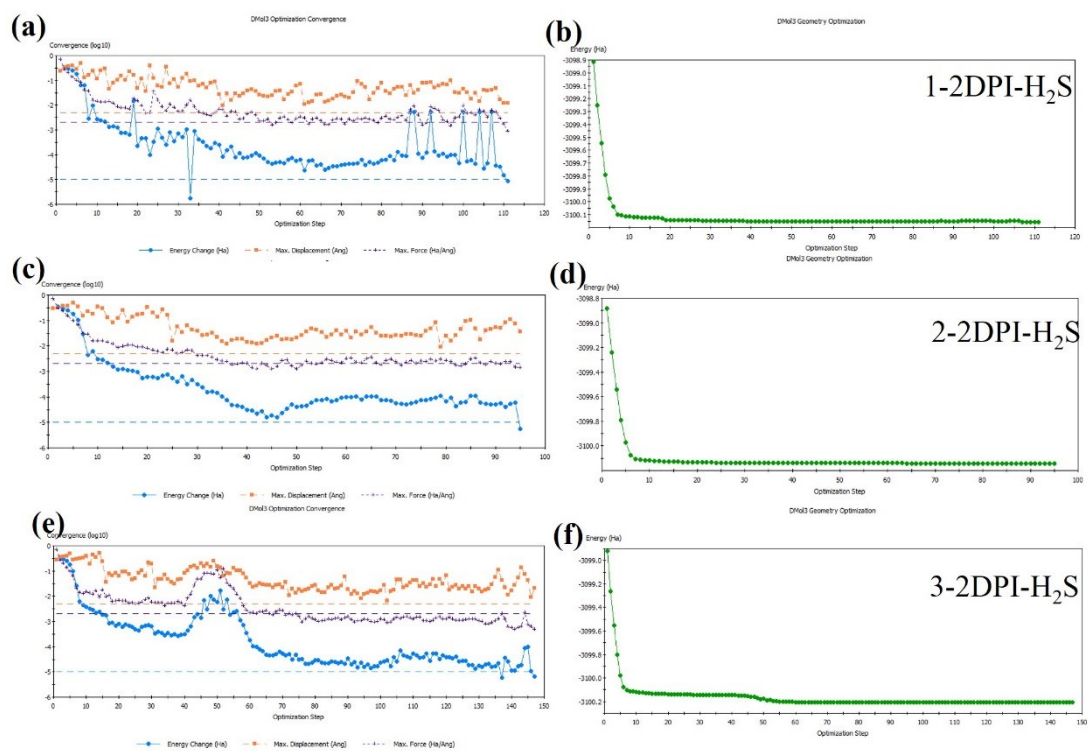


Figure S5. The relationship between convergence, energies and optimization step of H₂S adsorption system.

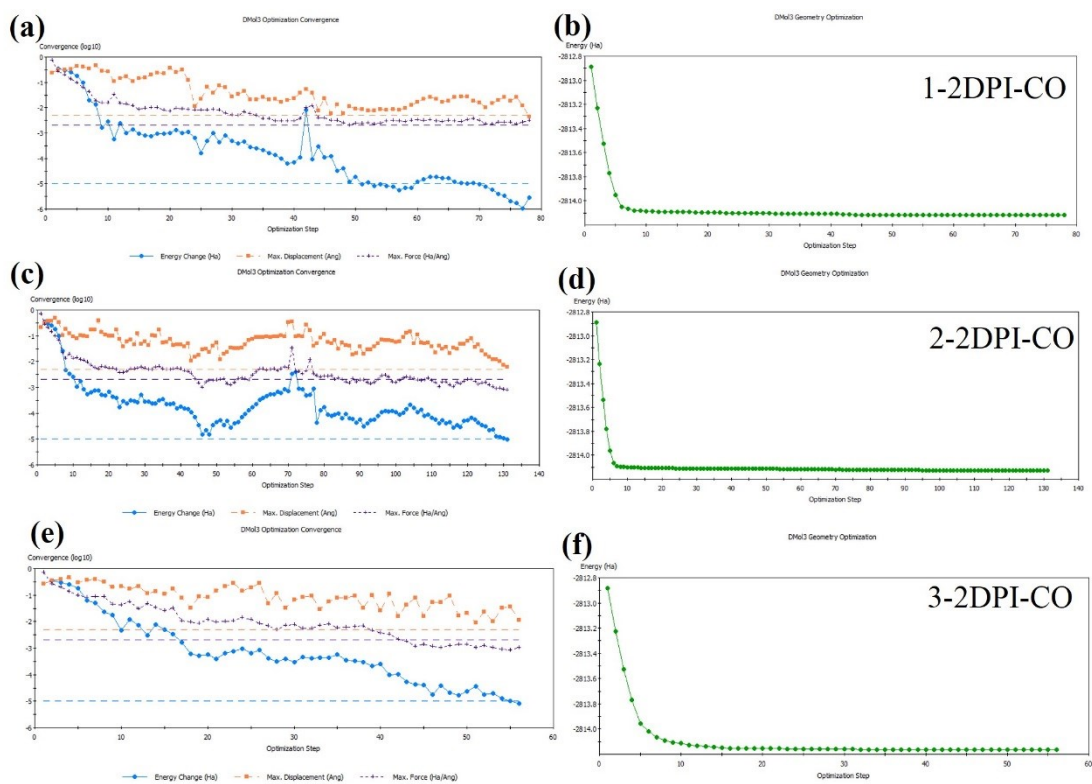


Figure S6. The relationship between convergence, energies and optimization step of CO adsorption system.