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菱形石墨炔薄膜 He 分离特性的密度泛函理论研究

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Helium Separation Performance of the Rhombic-Graphyne Monolayer Membrane: Density Functional Theory Calculations

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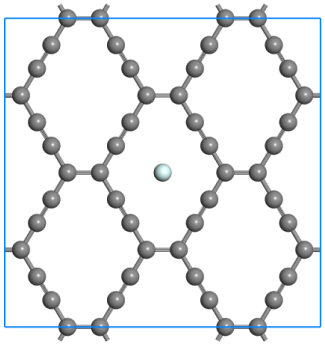
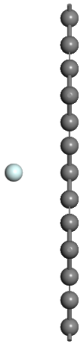
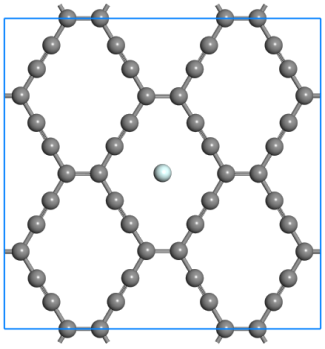
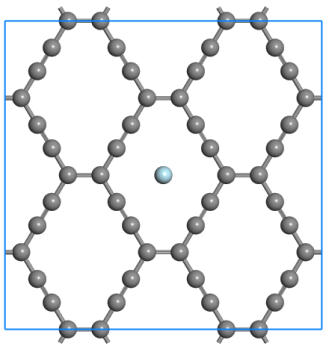
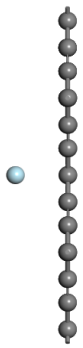
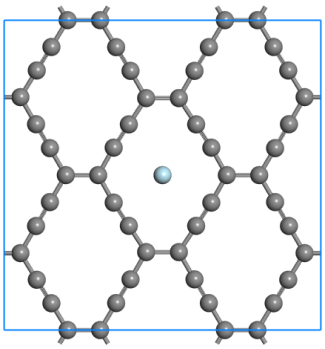
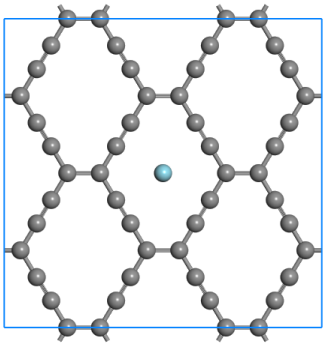
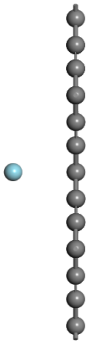
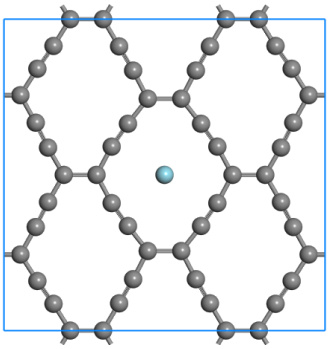
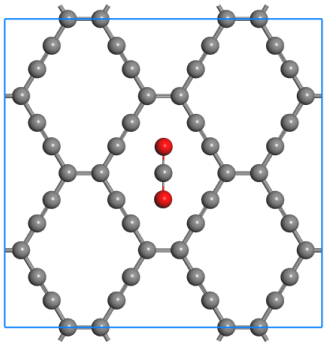
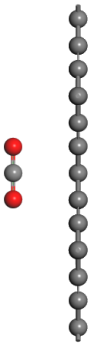
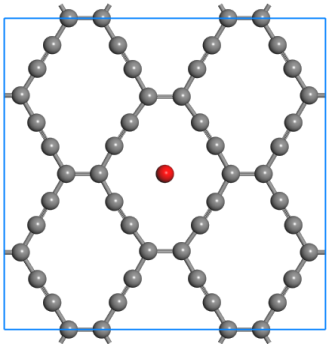
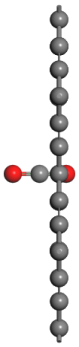
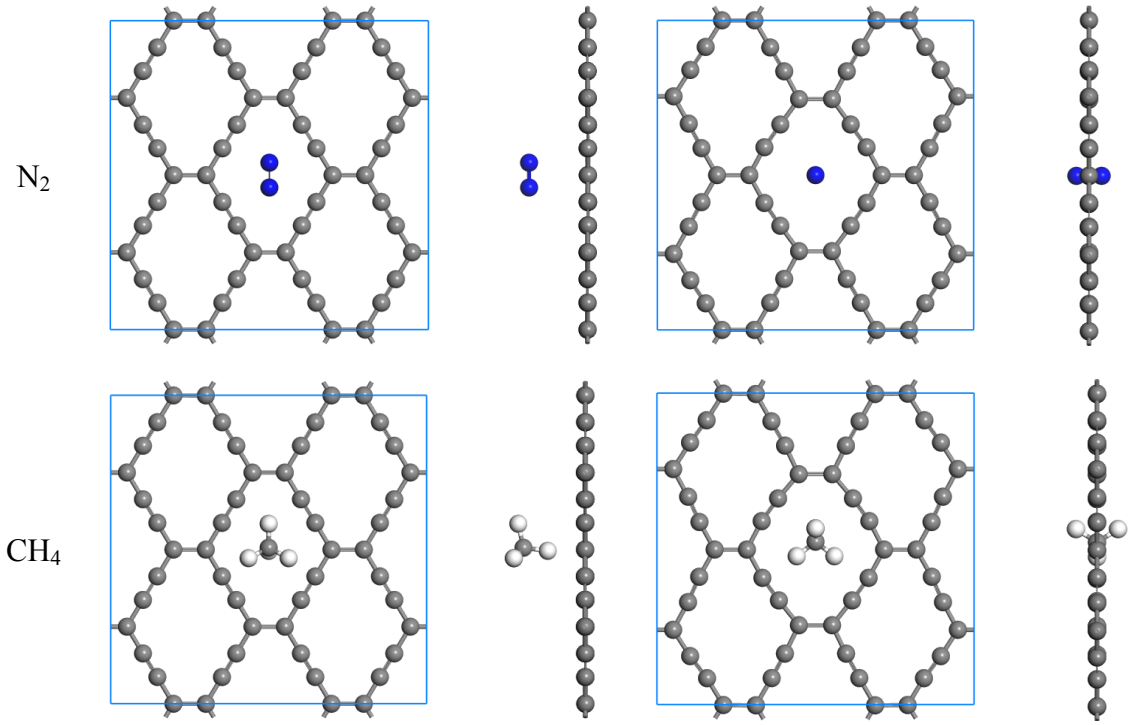
表 S1　各气体分子穿透 R-GY 分离膜过程中的吸附态和过渡态

Table S1　Adsorption states and transition states for the studied gases passing through the R-GY membrane.

	Adsorption state		Transition state	
	top view	side view	top view	side view
He				
Ne				
Ar				
CO_2				


N_2
CH_4