Supplementary Materials

$Mg_{12}O_{12}$ and $Be_{12}O_{12}$ Nanocages as Sorbents and Sensors for H_2S and SO_2 Gases: A Theoretical Approach

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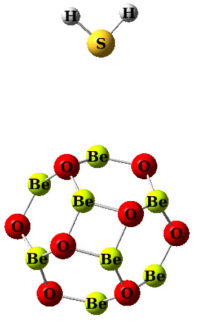
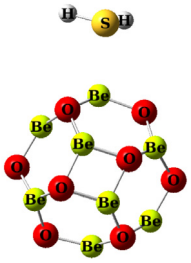
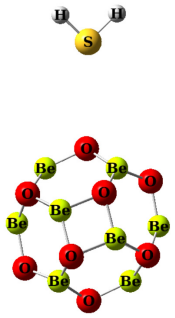
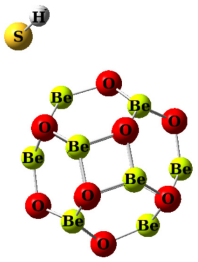
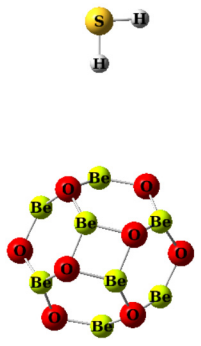
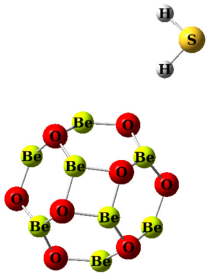
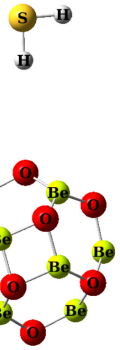
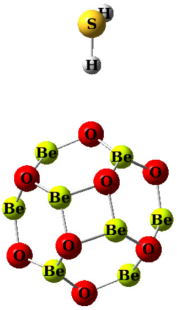
Table S1. The examined orientations for H_2S interaction with $Be_{12}O_{12}$.

mode	Input structure	Optimized structure	mode	Input structure	Optimized structure
1			5		
	E_{ads} = -0.31 eV			E_{ads} = -0.30 eV	
2			6		
	E_{ads} = -0.08 eV			E_{ads} = -0.09 eV	

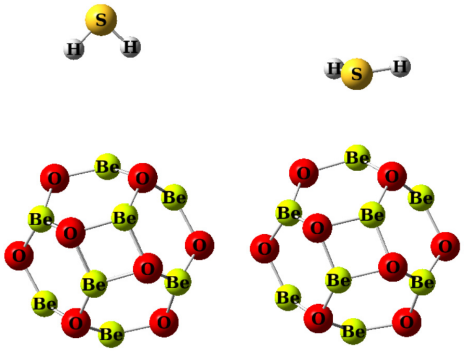
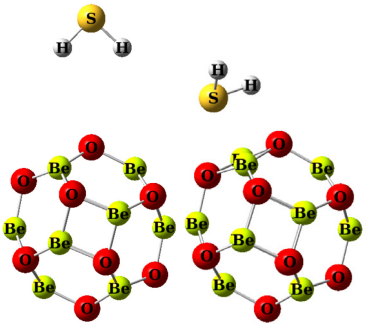
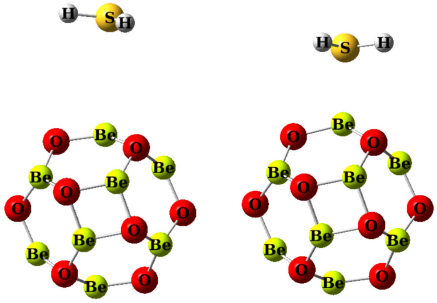
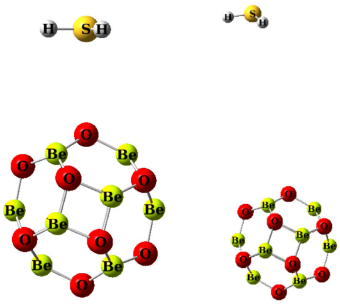
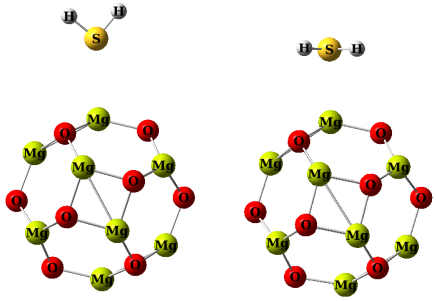
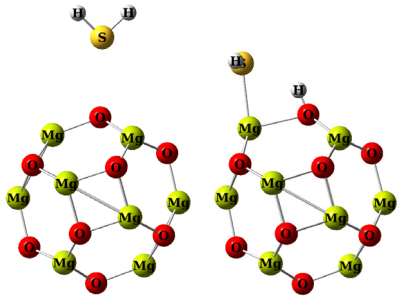
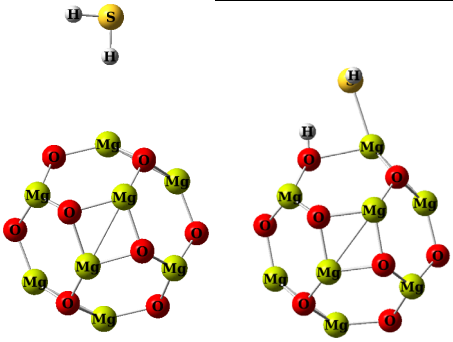
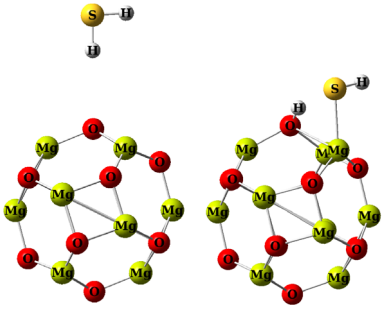
3		E_{ads} = -0.31 eV	7		E_{ads} = -0.31 eV
4		E_{ads} = -0.31 eV	8		E_{ads} = -0.01 eV

Table S2. The examined orientations for H_2S interaction with $Mg_{12}O_{12}$.

mode	Input structure	Optimized structure	mode	Input structure	Optimized structure
1		E_{ads} = -0.40 eV	5		E_{ads} = -1.24 eV
2			6		

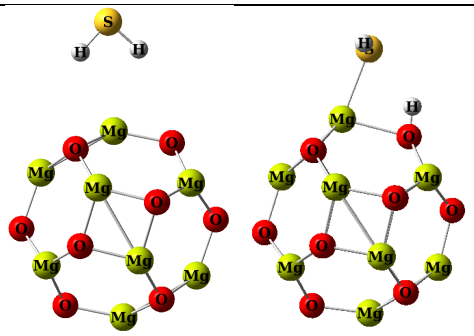
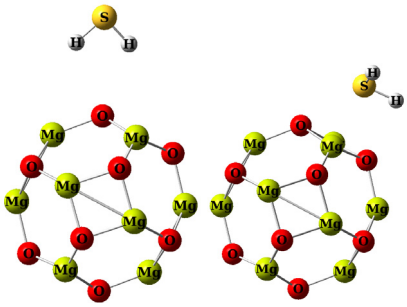
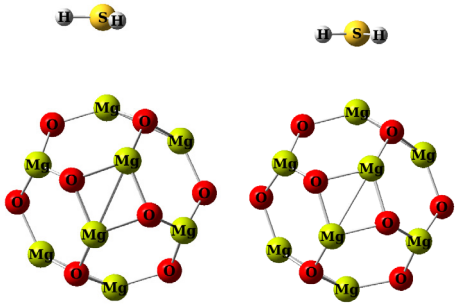
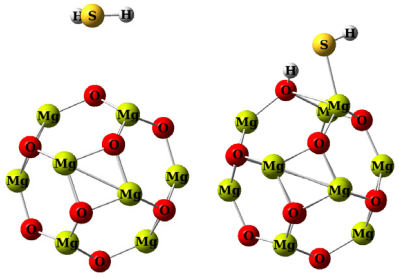
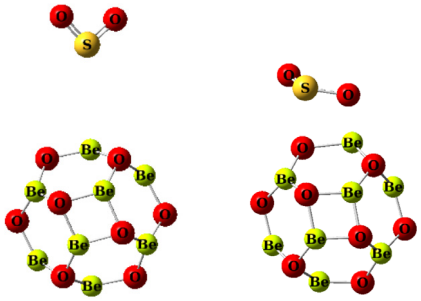
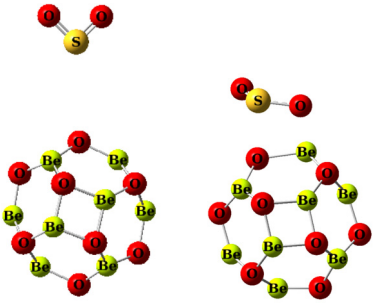
	E_{ads} = -1.25 eV	E_{ads} = -1.32 eV
3		7 
	E_{ads} = -1.25 eV	E_{ads} = -0.39 eV
4		8 
	E_{ads} = -0.39 eV	E_{ads} = -1.32 eV

Table S3. The examined orientations for SO_2 interaction with $Be_{12}O_{12}$.

mode	Input structure	Optimized structure	mode	Input structure	Optimized structure
1			5		
	E_{ads} = -0.56 eV			E_{ads} = -0.56 eV	

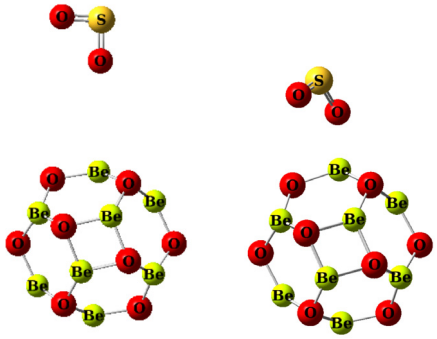
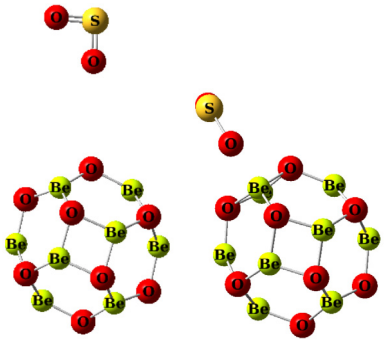
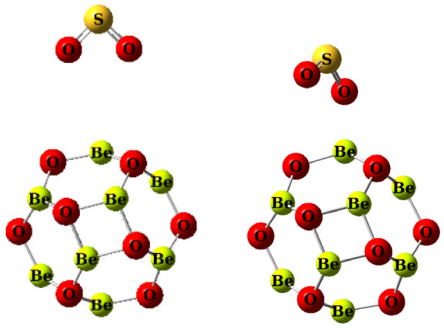
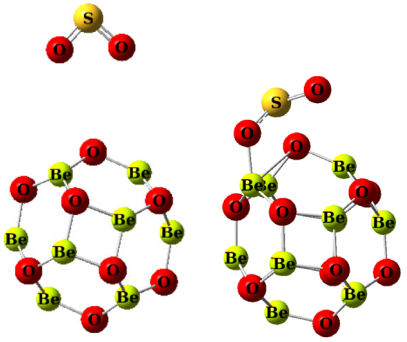
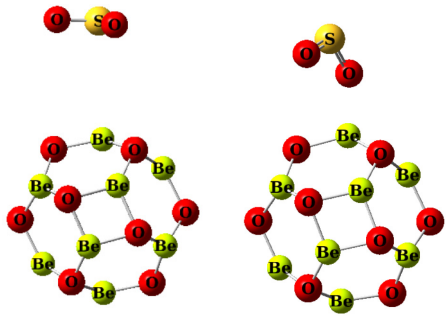
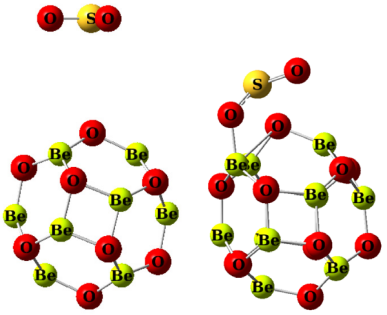
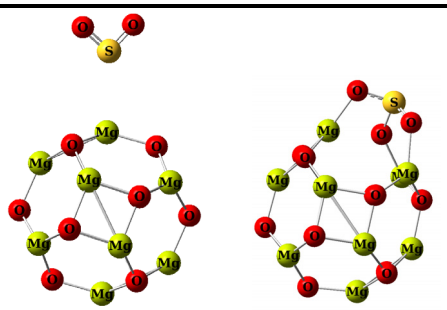
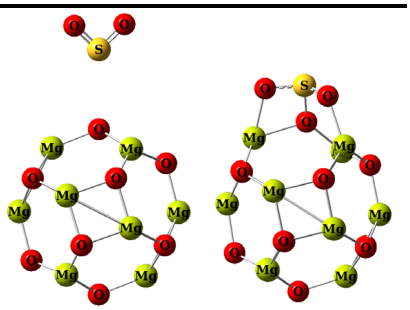
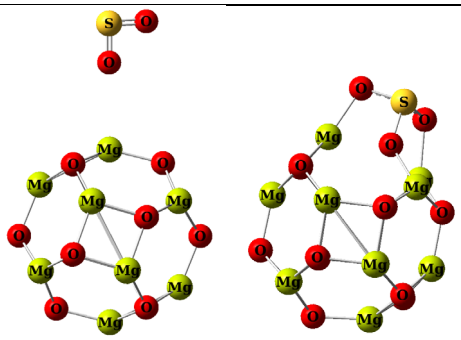
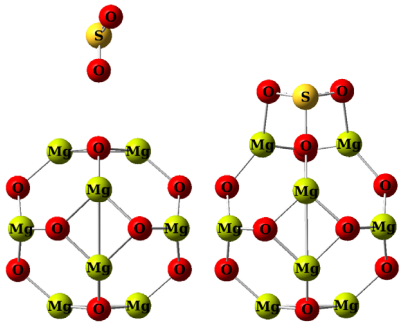
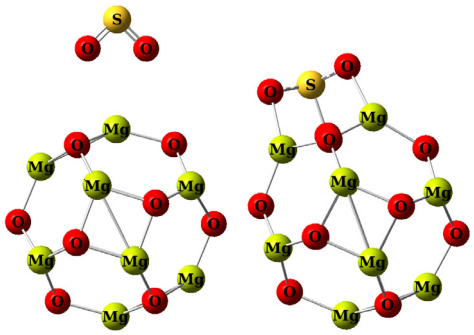
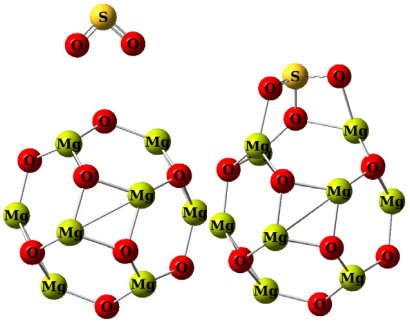
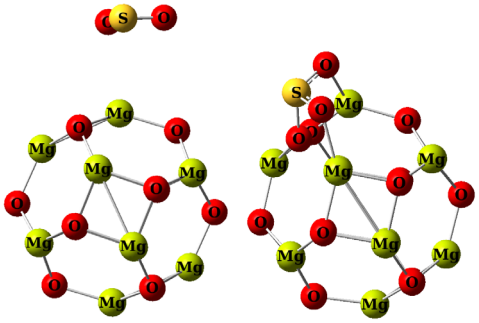
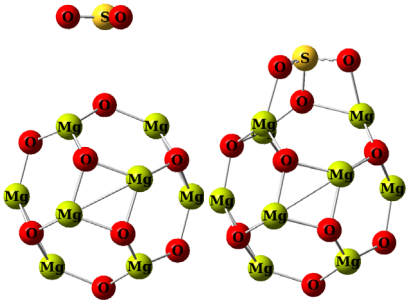
2		E_{ads} = -0.51 eV	6		E_{ads} = -0.51 eV
3		E_{ads} = -0.51 eV	7		E_{ads} = -0.83 eV
4		E_{ads} = -0.51 eV	8		E_{ads} = -0.83 eV

Table S4. The examined orientations for SO_2 interaction with $Mg_{12}O_{12}$.

mode	Input structure	Optimized structure	mode	Input structure	Optimized structure
1		E_{ads} = -2.33 eV	5		E_{ads} = -2.33 eV

2		E_{ads} = -2.32 eV	
6		E_{ads} = -2.29 eV	
3		E_{ads} = -2.28 eV	
7		E_{ads} = -2.32 eV	
4		E_{ads} = -2.32 eV	
8		E_{ads} = -2.32 eV	