Electronic Supplementary Information

Oxygen Adsorption on Single Layer Graphyne: A DFT Study

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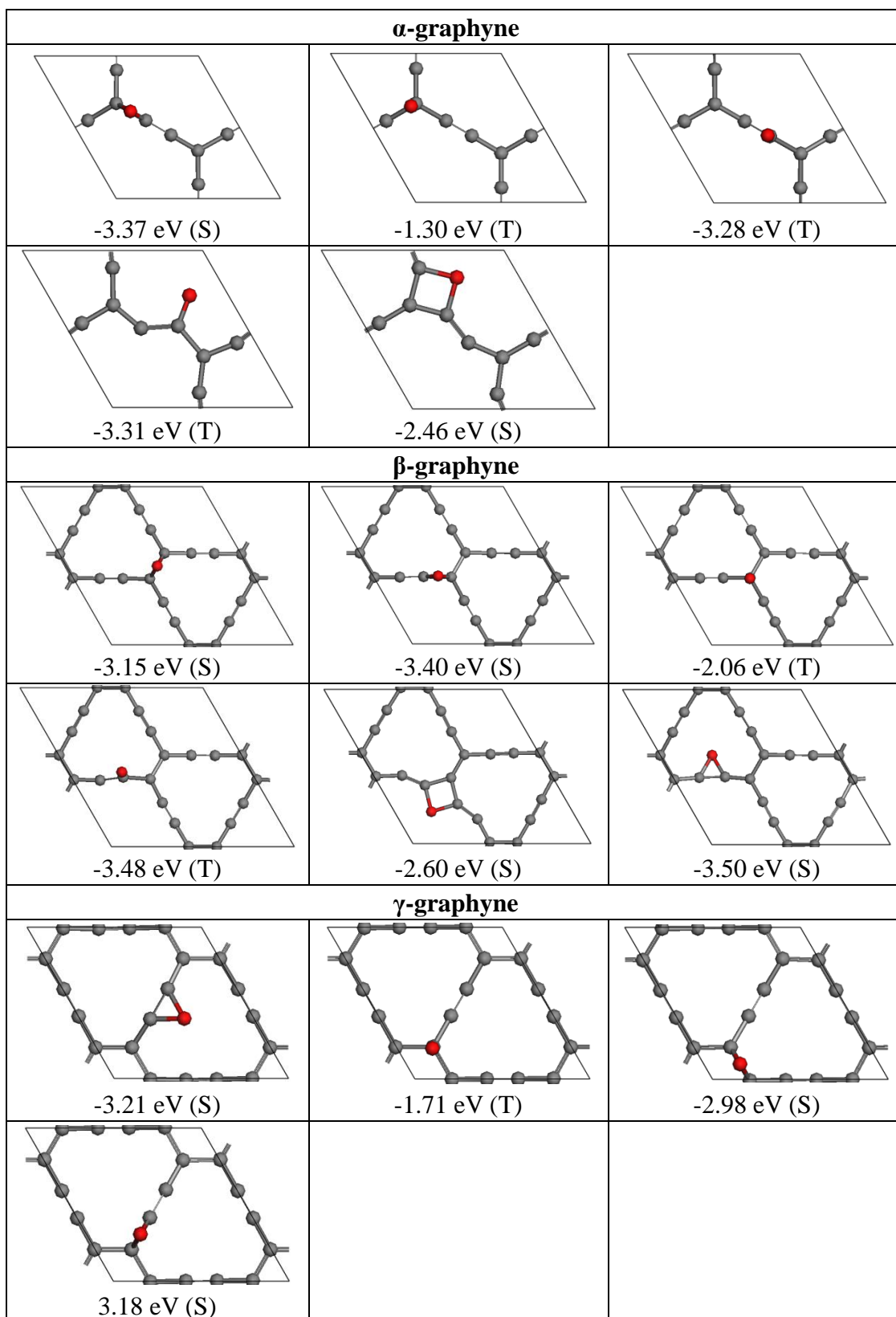Department of Chemistry, Sungkyunkwan University, Suwon, 440-746, Korea

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Table S1. The optimized lattice constant (a) and carbon-carbon bond lengths of each graphyne model obtained by LDA (PWC) method.

Figure S1. Oxygen binding sites for the α-, β- and γ-graphyne (S and T in parentheses stand for singlet and triplet state).

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	a(Å)	$R_{C1\text{-}C1}$(Å)	$R_{C1\text{-}C2}$(Å)	$R_{C2\text{-}C2}$(Å)	Band Gap (eV)
α-graphyne	6.920	1.226	1.384		0
β-graphyne	9.408	1.229	1.377	1.445	0
γ-graphyne	6.830	1.219	1.394	1.412	0.408

α-graphyne		
-3.37 eV (S)	-1.30 eV (T)	-3.28 eV (T)
-3.31 eV (T)	-2.46 eV (S)	
β-graphyne		
-3.15 eV (S)	-3.40 eV (S)	-2.06 eV (T)
-3.48 eV (T)	-2.60 eV (S)	-3.50 eV (S)
γ-graphyne		
-3.21 eV (S)	-1.71 eV (T)	-2.98 eV (S)
3.18 eV (S)		

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