**Supplementary Materials for: First-Principles Simulation of X-ray Spectra of Graphdiyne and Graphdiyne Oxides at the Carbon K-edge**

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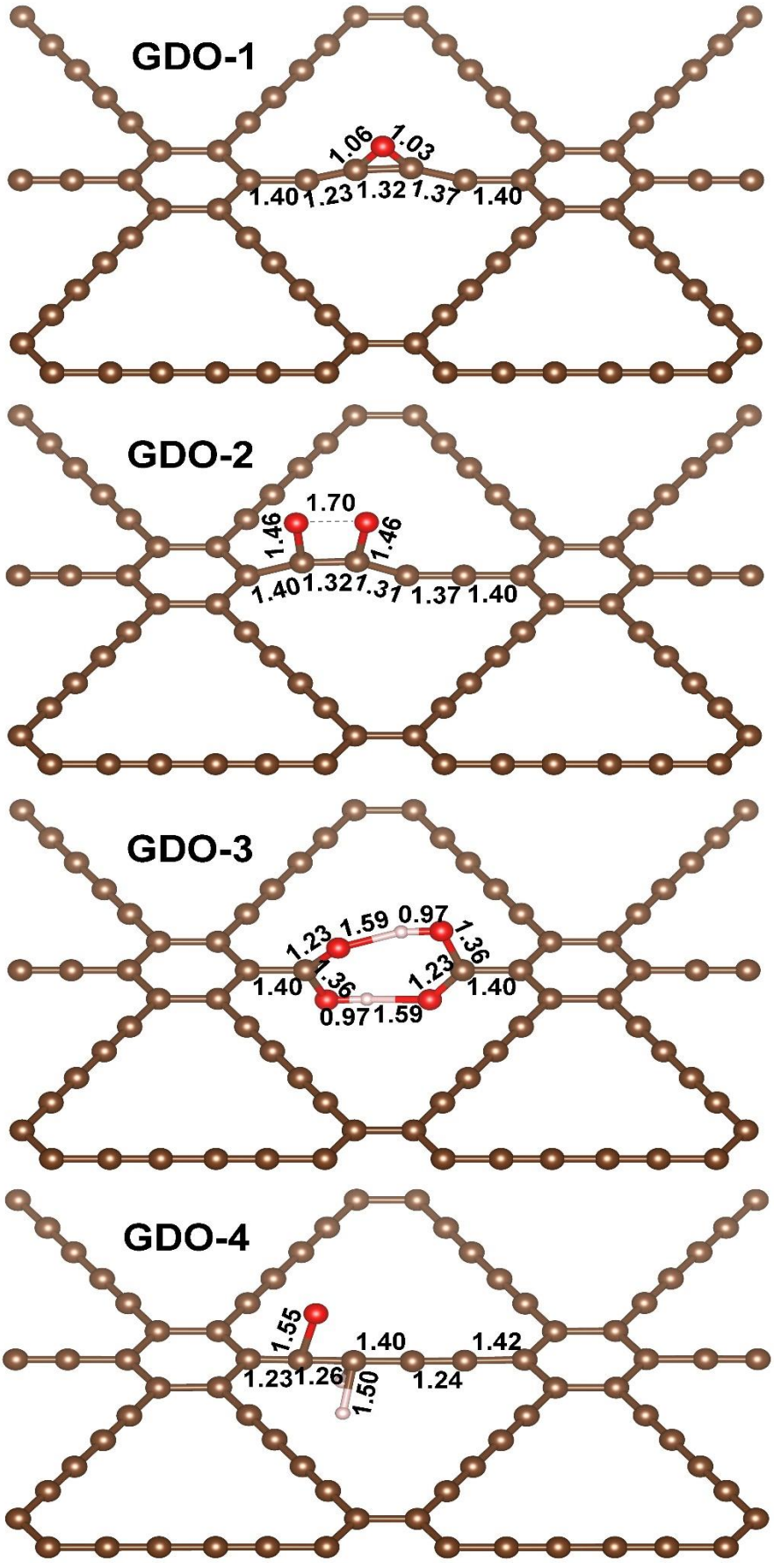


**Fig. S1.** The pre-optimization structures contain bond length (Å) information.

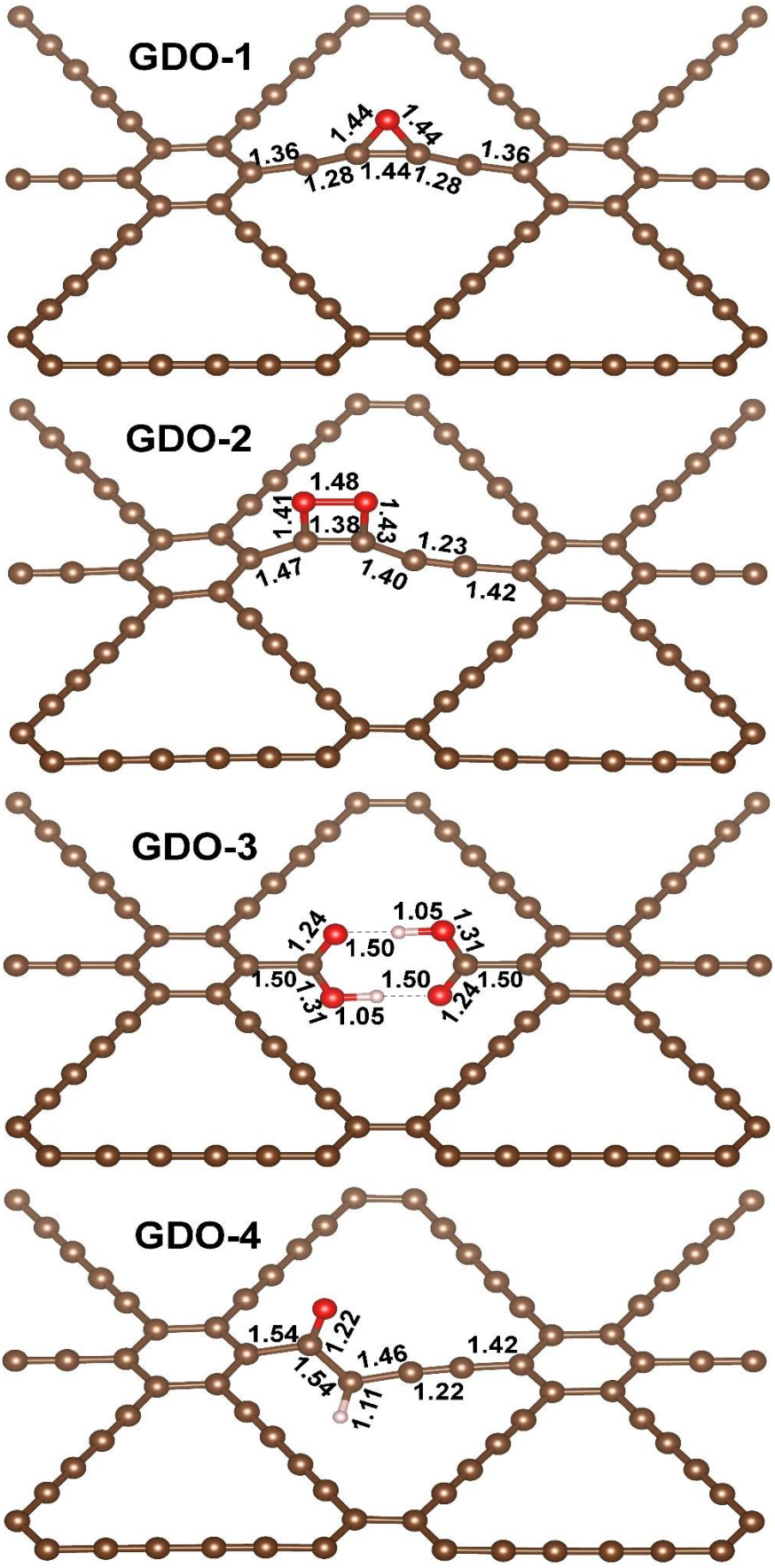


**Fig. S2.** The post-optimization structures contain bond length (Å) information.

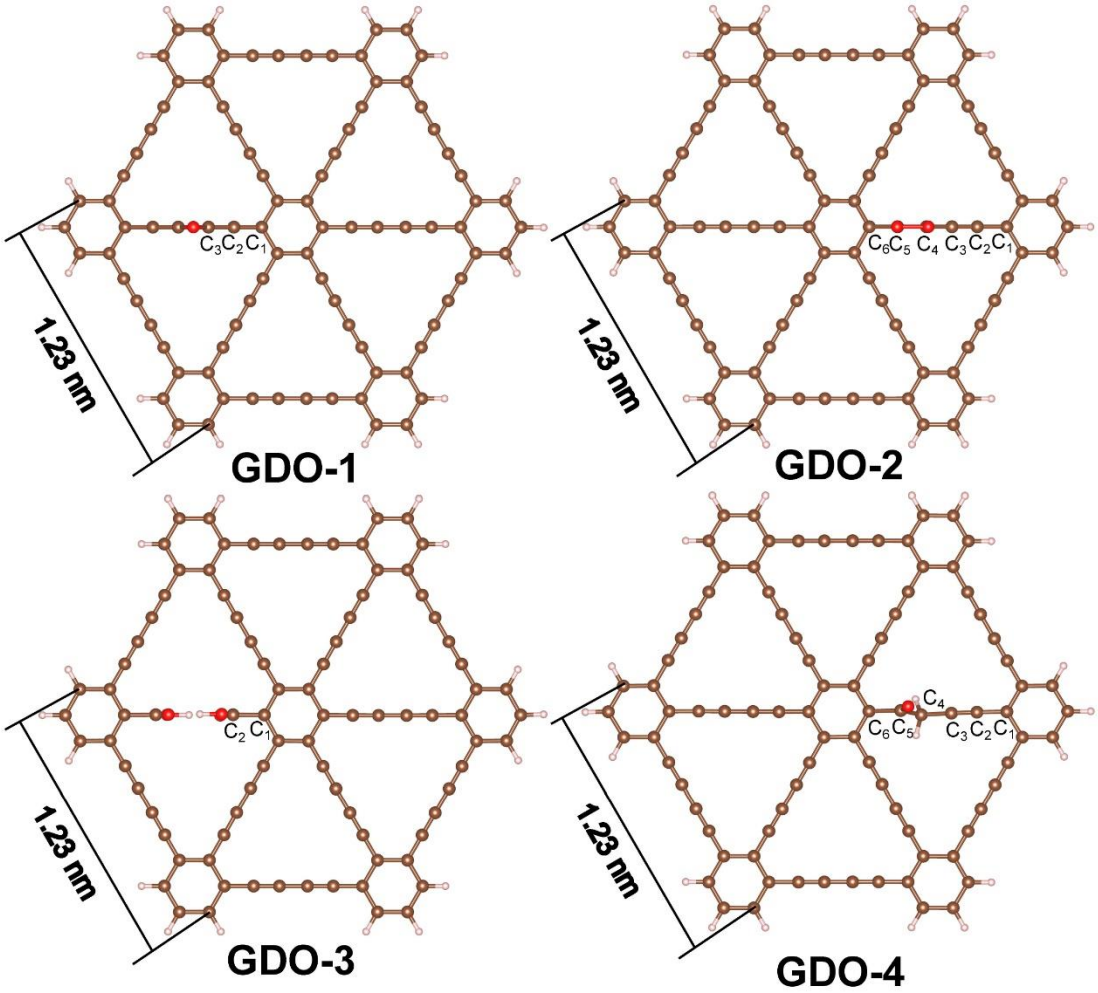


**Fig. S3.** Cluster models used to calculate the IPs for four different graphdiyne oxides (GDOs) and their sizes are labeled. The excited atoms are labeled $C_1$, $C_2$, $C_3$ ……

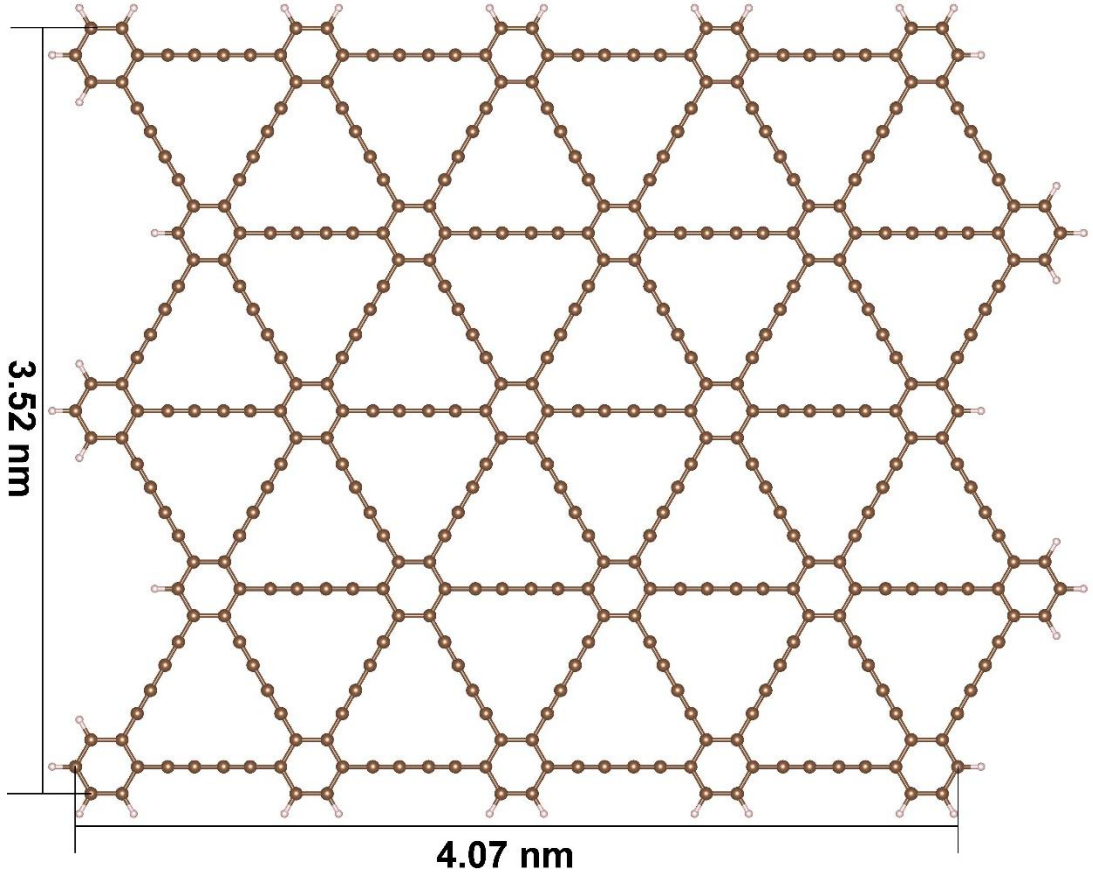


**Fig. S4.** Size B: the vertical length of GDY is 3.52nm between the bottom carbon atoms and the top carbon atoms; the parallel length of GDY is 4.07nm from the left carbon atoms to the right carbon atoms.

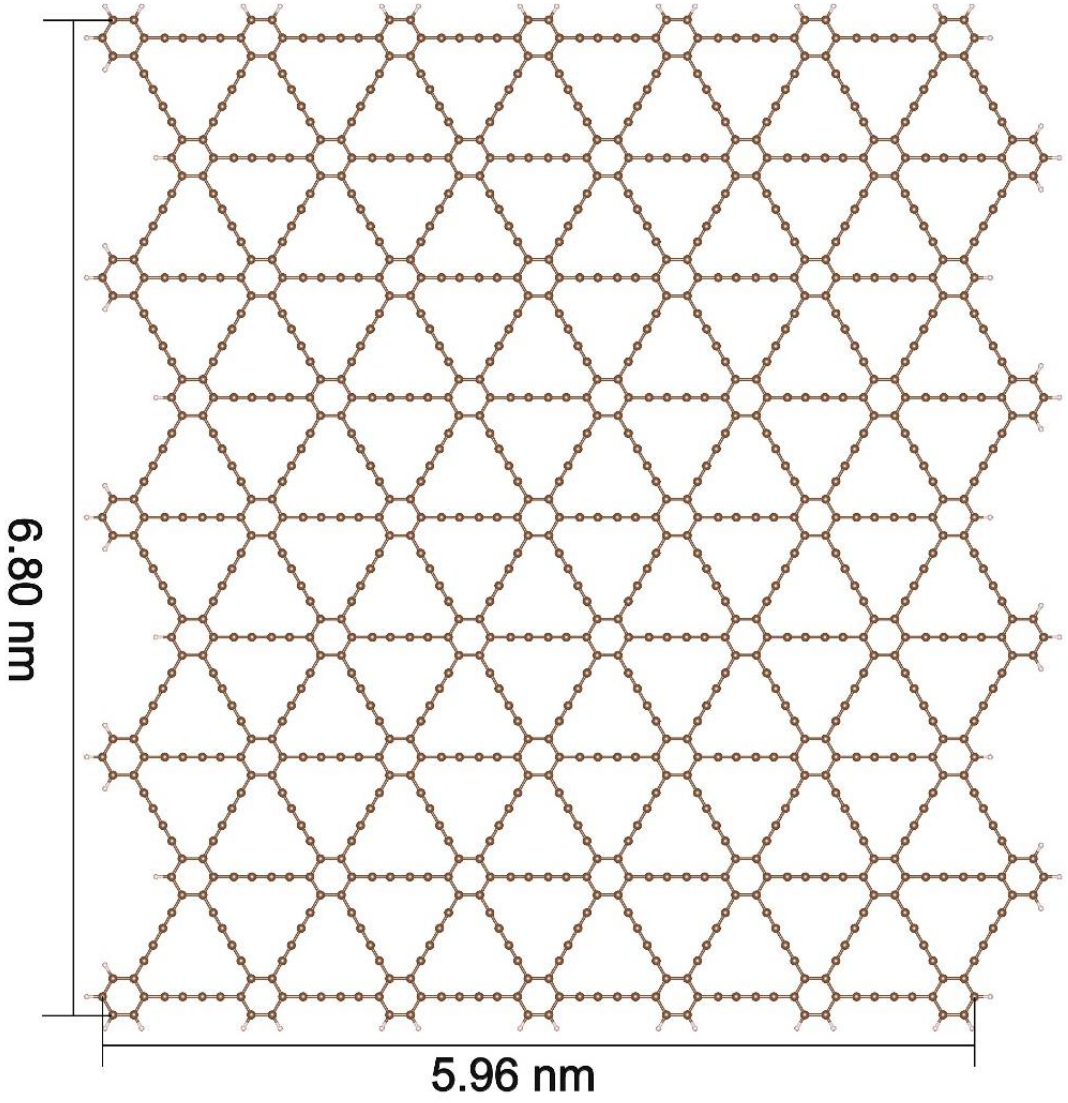


**Fig. S5.** Size D with 6.80nm of the vertical length and 5.96nm of the parallel length similar to Fig. S2.