Supplementary Information for: Towards sensitive identification of fluorinated graphdiyne configurations by computational X-ray spectroscopy.

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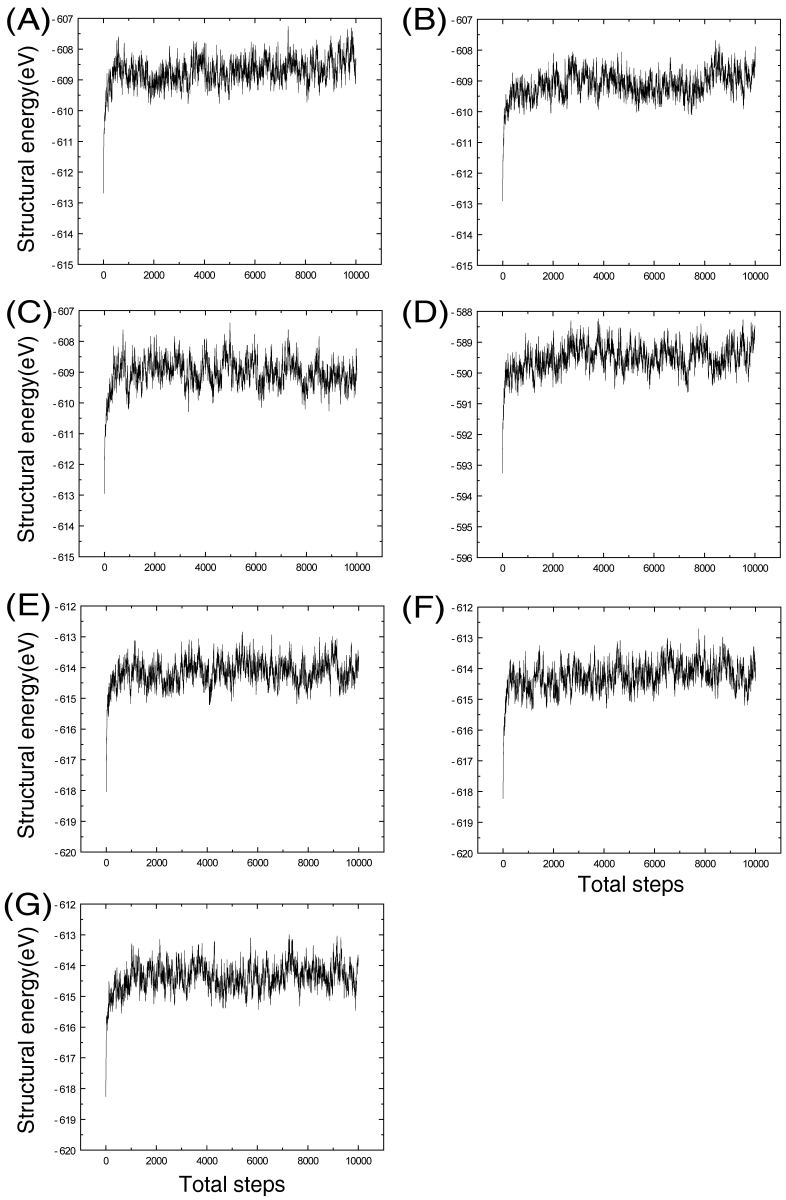

Figure S1. The ab initio molecular dynamics (AIMD) production run of seven fluorinated graphdiynes at 300 K, and structural energy of the computational cell on the simulation time after AIMD were shown in the corresponding graph.

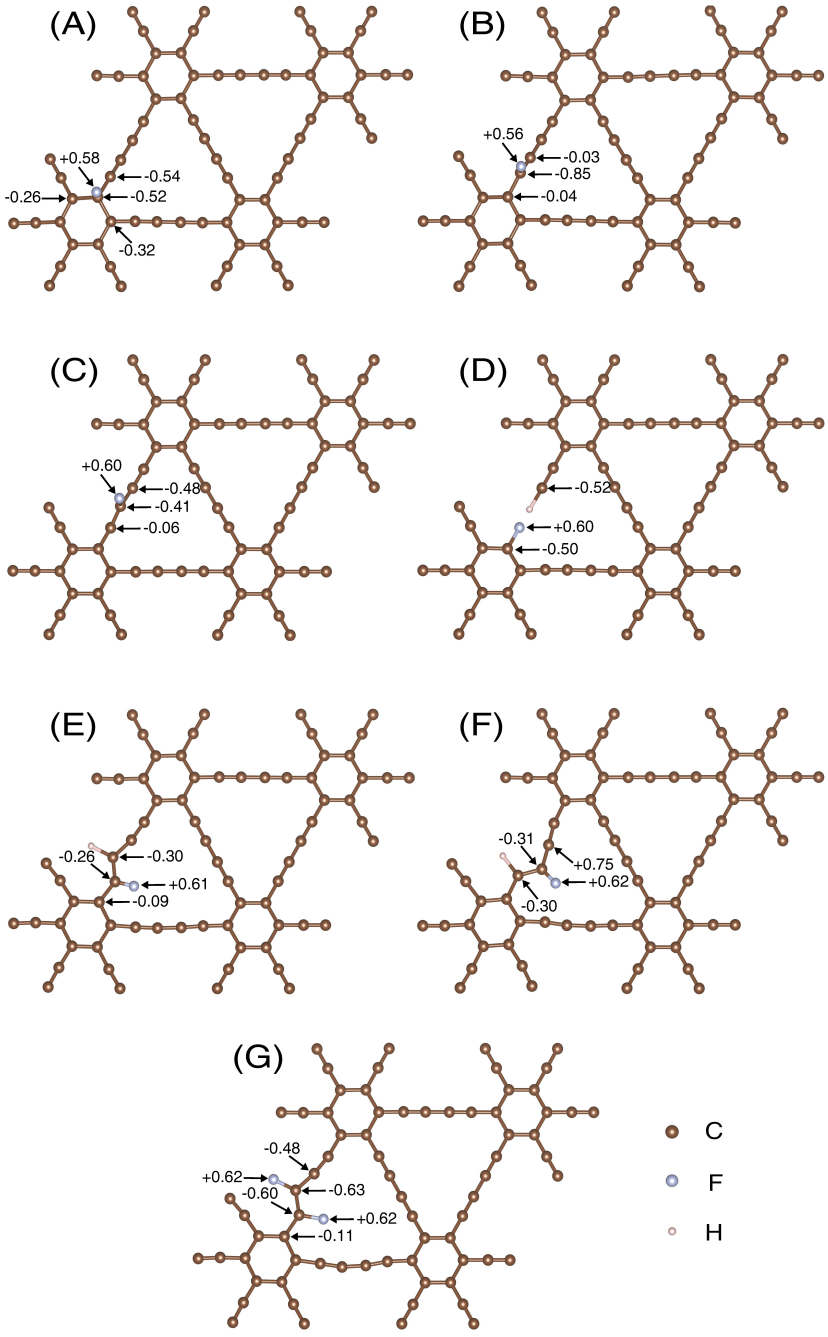

Figure S2. Bader effective charge analysis of fluorine atoms and adjacent carbon atoms for all the configurations. Positive and negative values represent

the number of electrons obtained and lost, respectively.