Supplementary Information for

Chemical properties of superatomic Li_3O clusters from density functional theory perspective: formation of chloride and adsorption behavior on graphynes

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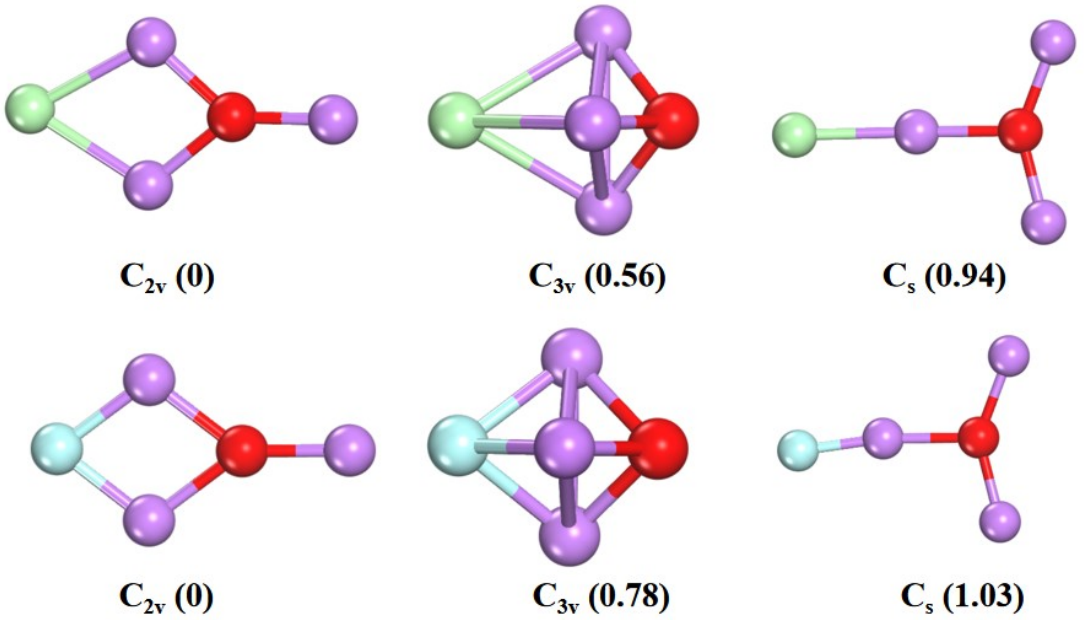

Figure S1. The lowest energy structures and the metastable isomers of the $Li_3O(Cl)$ and $Li_3O(F)$ halides. Numbers in the brackets are the energies (in eV) of the clusters relative to the lowest energy energies. Green, blue and red spheres represent chlorine, fluorine and oxygen atoms, respectively. Space groups were determined with a tolerance of 0.1 Å.