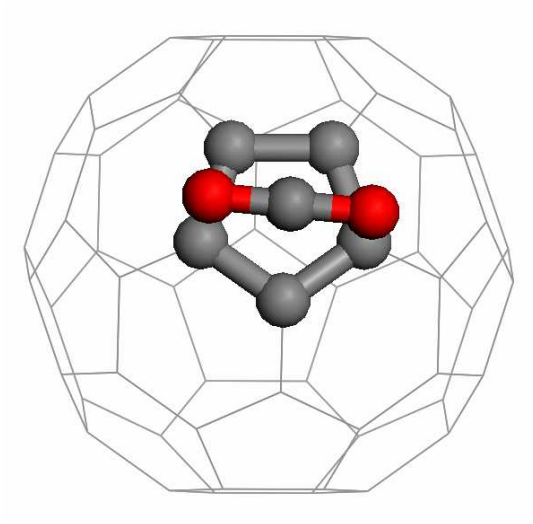
## Supporting Information

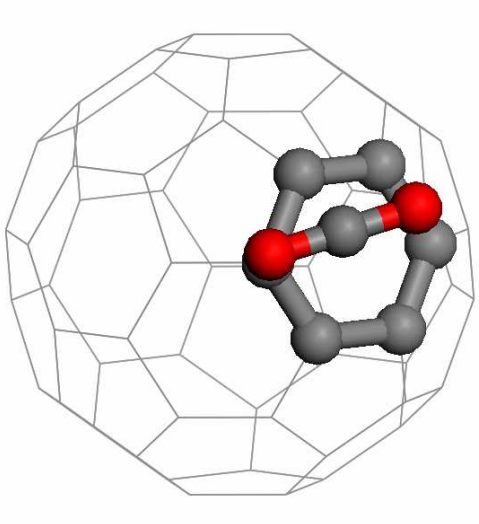
**Figure S1.** Optimized structures for the $CO_2$ molecules adsorbed on the (a) hexagon, (b) pentagon, and (c) bond sites in pristine $C_{60}$.

**Figure S2.** Optimized structures for a single Ca atom adsorbed on pristine $C_{60}$ on (a) pentagon, (b) hexagon sites in pristine $C_{60}$. (c) The projected density of states of Ca atom in Ca-doped $C_{60}$ complex. The bond distances are in angstroms.

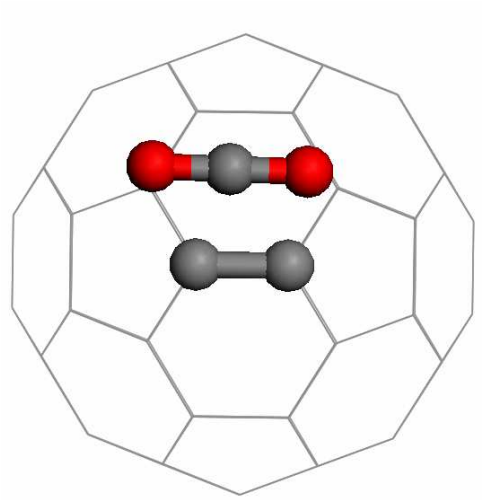
**Figure S1**



(a)

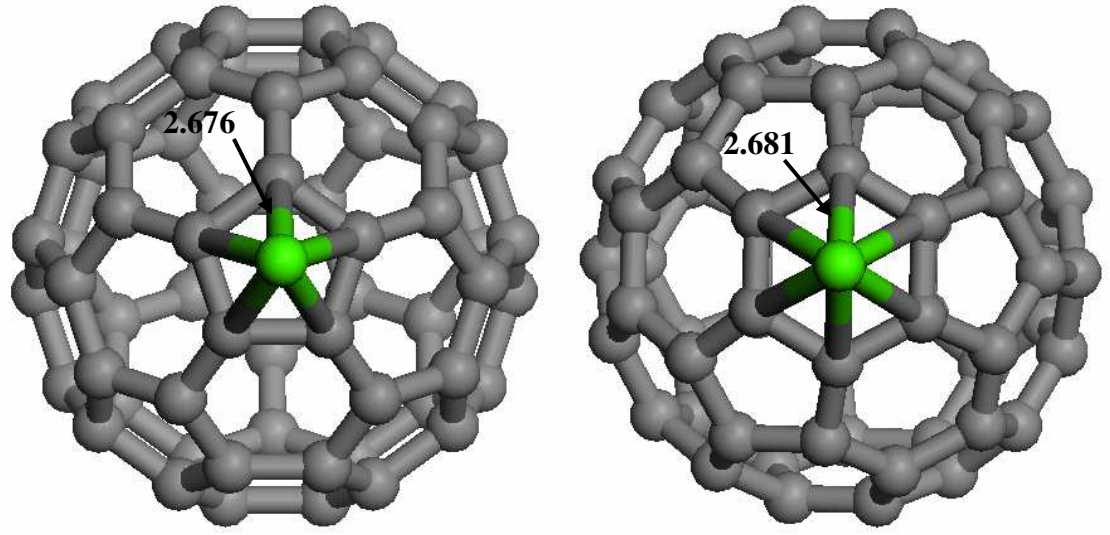


(b)

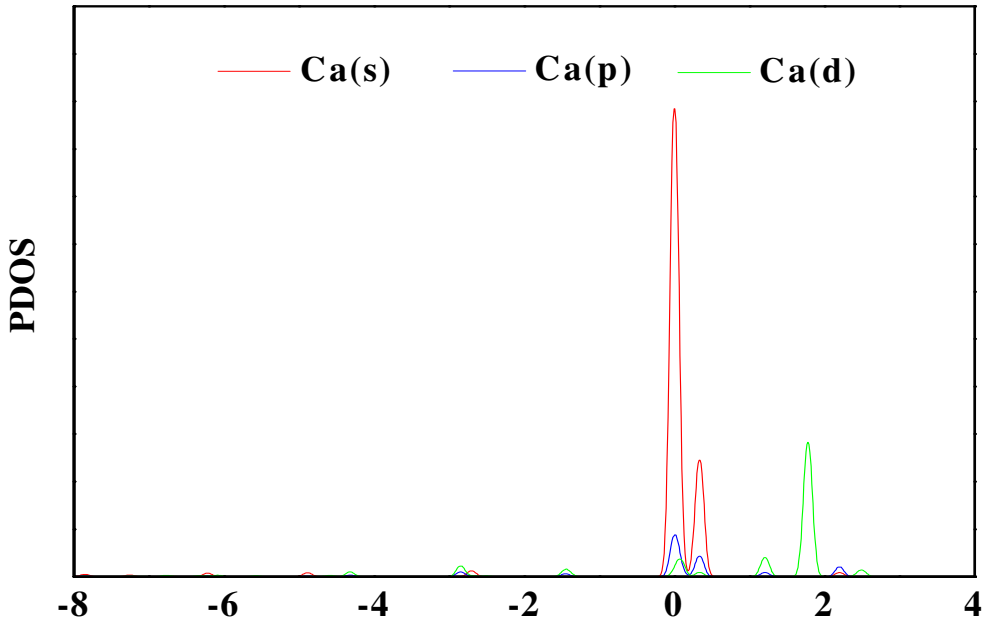


(c)

**Figure S2**




(a) $E_{ads}$ = -1.487 eV (b) $E_{ads}$ = -1.431 eV




(c)