# Supplementary Information

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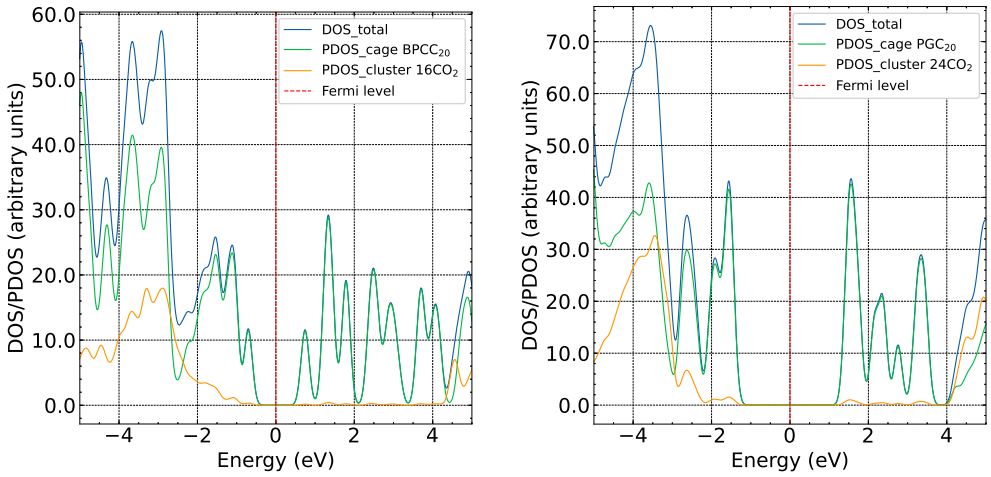
## 1 DOS and PDOS

The Density of States, or DOS, of a system describes the number of electronic states available to be occupied by electrons at a given energy level.

Tests were performed to determine the system's DOS and PDO). The results were obtained from calculations performed with the DFTB+ software. Having the DOS curve, it is possible to quantify how much the cluster influences the distribution of system states.

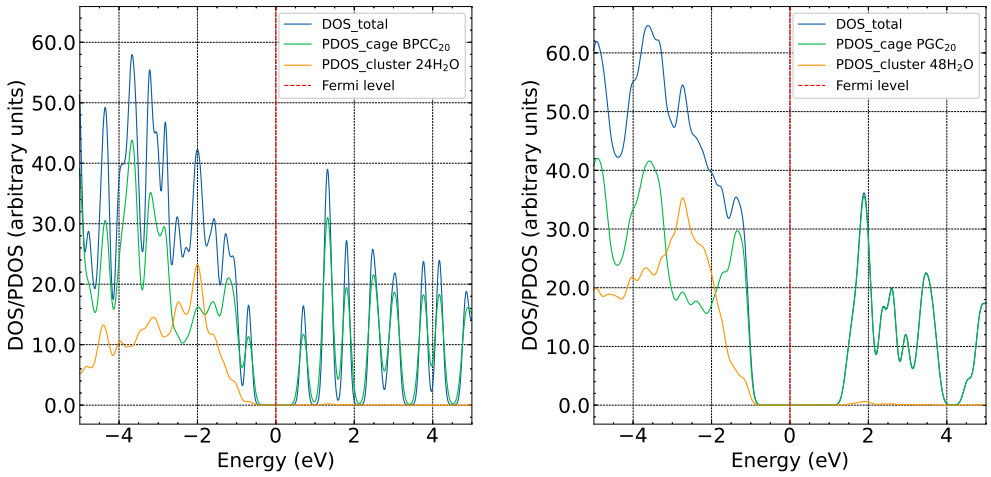
The graphs in Figure 1, Figure 2 and Figure 3, indicates the DOS and PDOS for the systems at maximum capacities for the fullerenes $BPCC_{20}$ and $PGC_{20}$. For the three types of molecules $CO_2$, $H_2O$ and $H_2$, respectively. Negative energies correspond to occupied electronic states, and positive energies correspond to unoccupied states.

In cases where the clusters are encapsulated in a BPC cage, the results indicate that the conduction band is almost exclusively contributed by the cage, which means that the lowest-energy unoccupied electronic states belong to the structure, not to the encapsulated molecules. The case is repeated with the clusters encapsulated in PG cage, with the exception of the $58H_2@PGC_{20}$ system, where the gas molecules significantly influence the conduction band. In all systems the valence band presents a mixed contribution from cluster and cage.



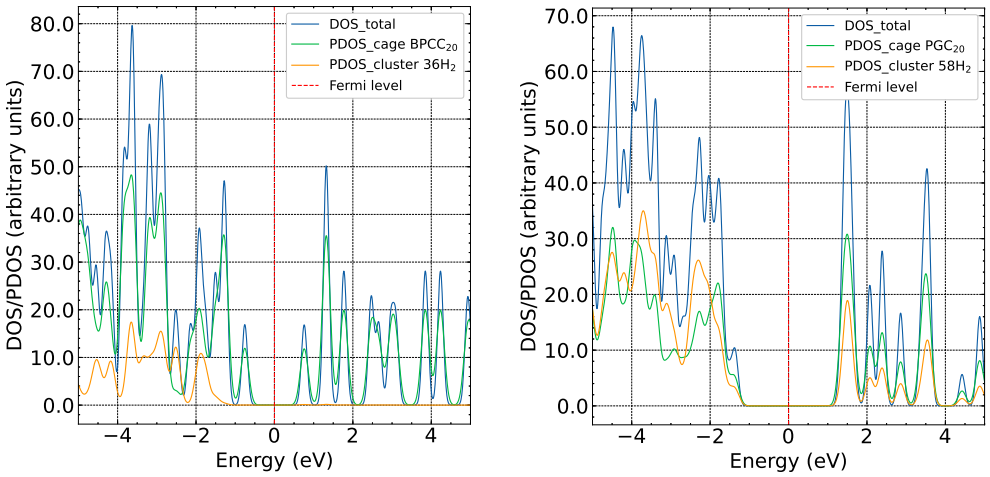

(a) (b)

**Fig. 1**: (a) $16CO_2$@$BPCC_{20}$ and (b) $24CO_2$@$PGC_{20}$. The red dashed line represents the Fermi level. The blue curve represents the total system DOS. The orange and green curves represent the cluster and cage contribution PDOS, respectively.




(a) (b)

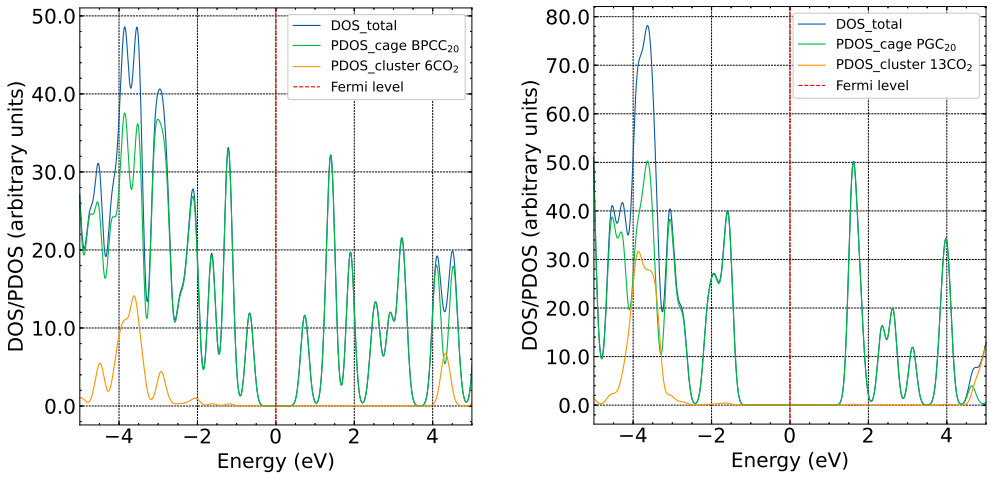
**Fig. 2**: (a) $24H_2O$@$BPCC_{20}$ and (b) $48H_2O$@$PGC_{20}$. The red dashed line represents the Fermi level. The blue curve represents the total system DOS. The orange and green curves represent the cluster and cage contribution PDOS, respectively.




(a) (b)

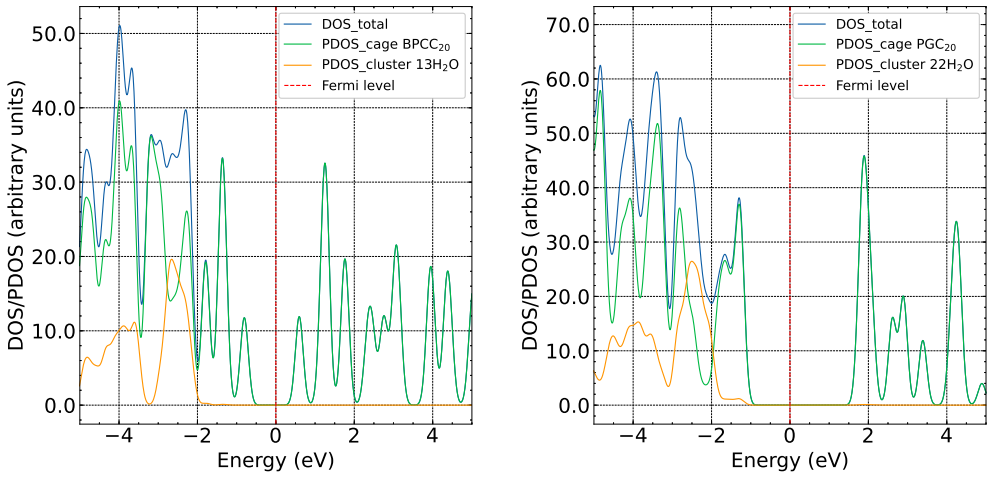
**Fig. 3**: (a) $36H_2$@$BPCC_{20}$ and (b) $58H_2$@$PGC_{20}$.The red dashed line represents the Fermi level. The blue curve represents the total system DOS. The orange and green curves represent the cluster and cage contribution PDOS, respectively.

The same considerations apply to the stable systems indicated in Figure 4, Figure 5 and Figure 6. The graphs represent, respectively, the stable systems $6CO_2$@$BPCC_{20}$, $13CO_2$@$PGC_{20}$, $13H_2O$@$BPCC_{20}$, $22H_2O$@$PGC_{20}$, $13H_2$@$BPCC_{20}$ and $20H_2$@$PGC_{20}$.



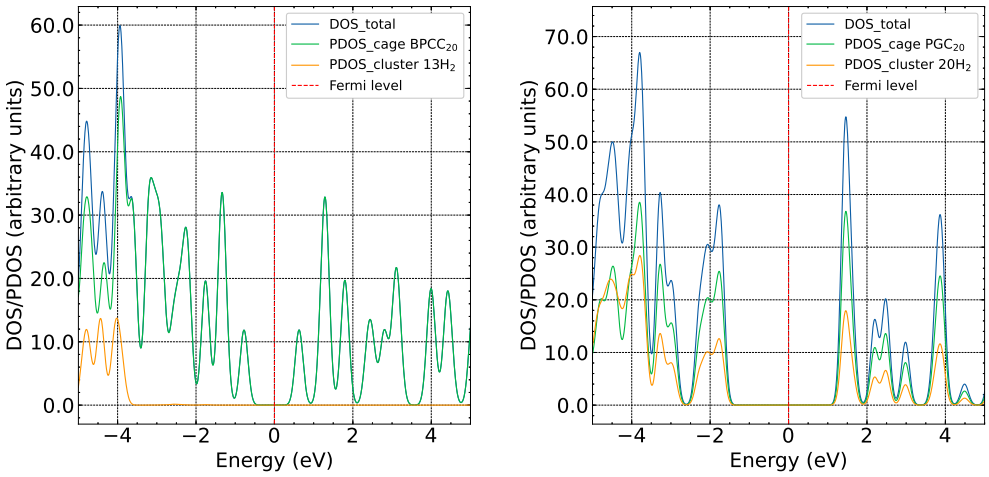

(a) (b)

**Fig. 4**: (a) $6CO_2$@$BPCC_{20}$ and (b) $13CO_2$@$PGC_{20}$. The red dashed line represents the Fermi level. The blue curve represents the total system DOS. The orange and green curves represent the cluster and cage contribution PDOS, respectively.




(a) (b)

**Fig. 5**: (a) $13H_2O$@$BPCC_{20}$ and (b) $22H_2O$@$PGC_{20}$. The red dashed line represents the Fermi level. The blue curve represents the total system DOS. The orange and green curves represent the cluster and cage contribution PDOS, respectively.




(a) (b)

**Fig. 6**: (a) $13H_2$@$BPCC_{20}$ and (b) $20H_2$@$PGC_{20}$.The red dashed line represents the Fermi level. The blue curve represents the total system DOS. The orange and green curves represent the cluster and cage contribution PDOS, respectively.

## 2 Radial Distribution $g(r)$

The radial distribution $g(r)$ shown in the main text represents the distances between molecules in the clusters within the cages. Other distributions were computed using VMD software. Since $C_2$2 and $H_2O$ molecules each have two distinct atoms, the distribution for the distance between the molecules and each of the atoms that make up these molecules was calculated. In Figure 7, Figure 8, Figure 9 and Figure 10 we can observe these effects. These graphs show that even in systems with maximum capacity, the formation distances between the atoms of the gas molecules were maintained.

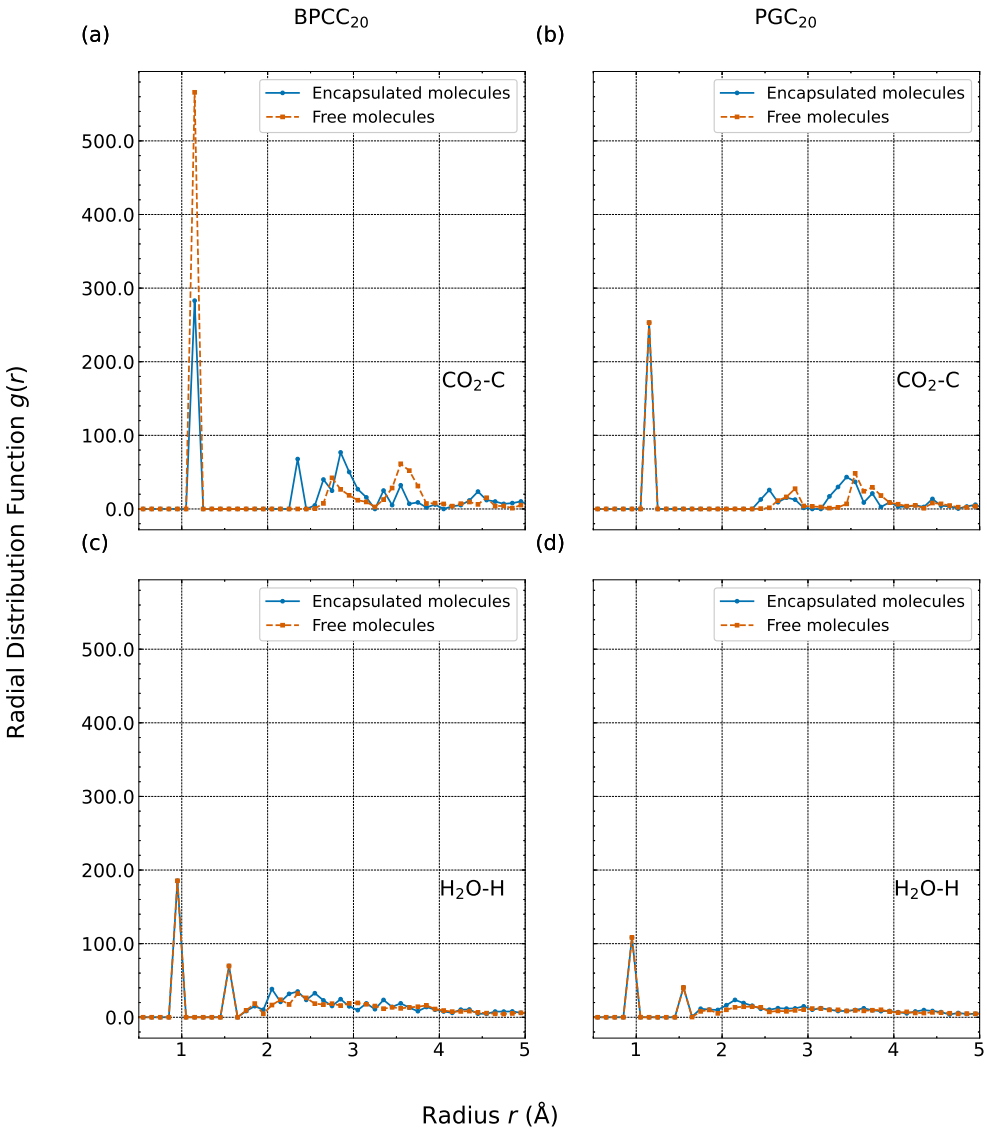



**Fig. 7**: Radial distribution in stable systems for the distances between $CO_2$ and carbon atom in (a) $BPCC_{20}$ and (b) $PGC_{20}$, and distances between $H_2O$ and hydrogen atom in (c) $BPCC_{20}$ and (d) $PGC_{20}$.

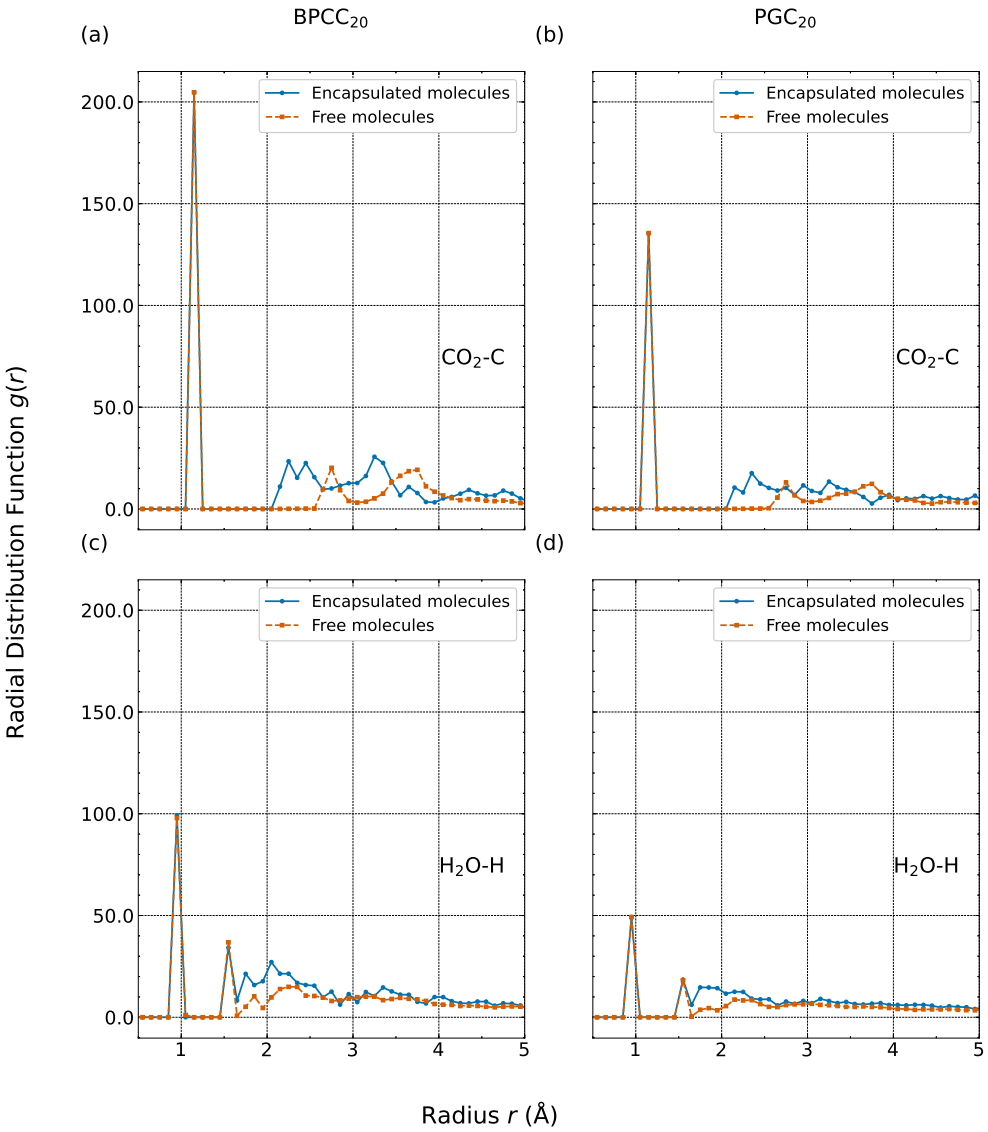



**Fig. 8**: Radial distribution in maximum systems for the distances between $CO_2$ and carbon atom in (a) $BPCC_{20}$ and (b) $PGC_{20}$, and distances between $H_2O$ and hydrogen atom in (c) $BPCC_{20}$ and (d) $PGC_{20}$.

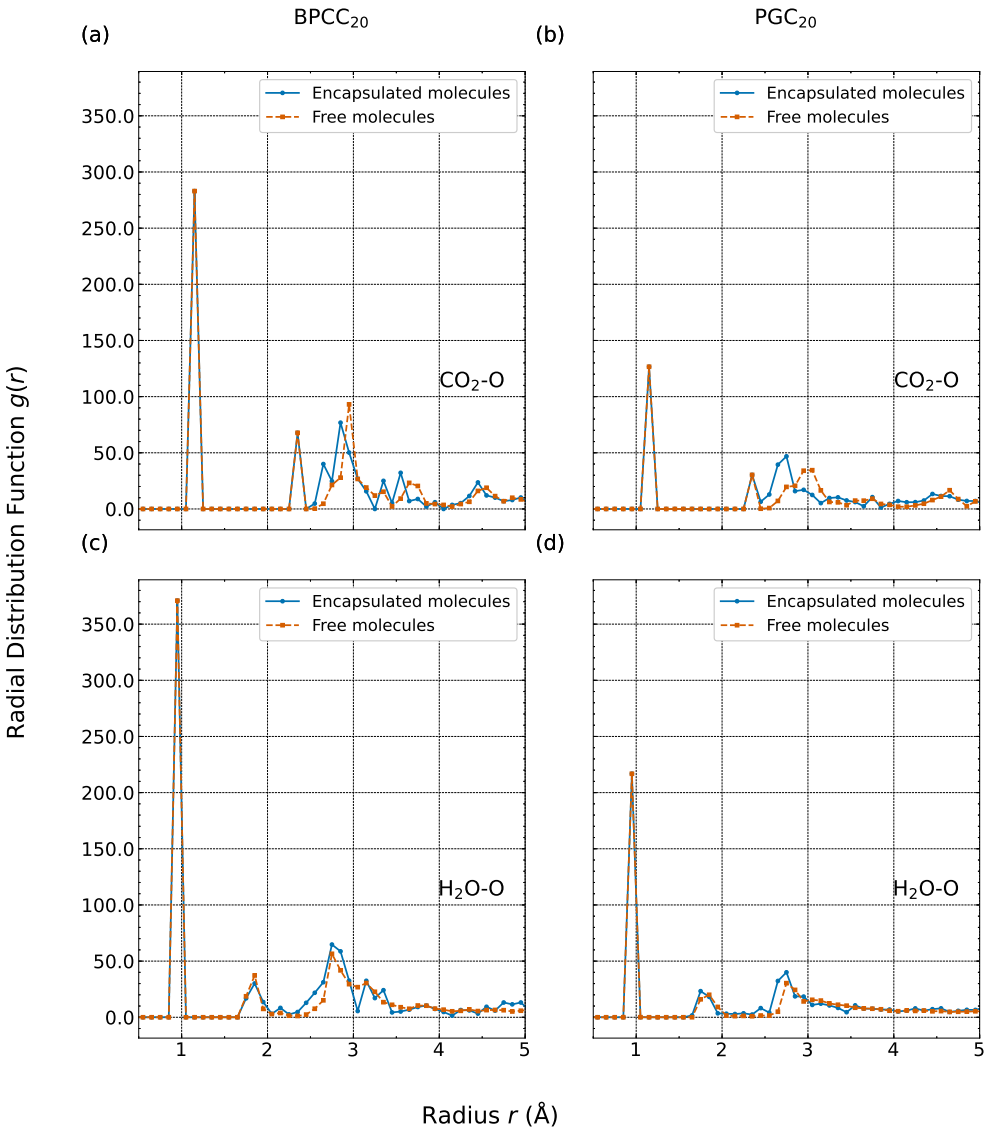



**Fig. 9**: Radial distribution in stable systems for the distances between $CO_2$ and oxygen atom in (a) $BPCC_{20}$ and (b) $PGC_{20}$, and distances between $H_2O$ and oxygen atom in (c) $BPCC_{20}$ and (d) $PGC_{20}$.

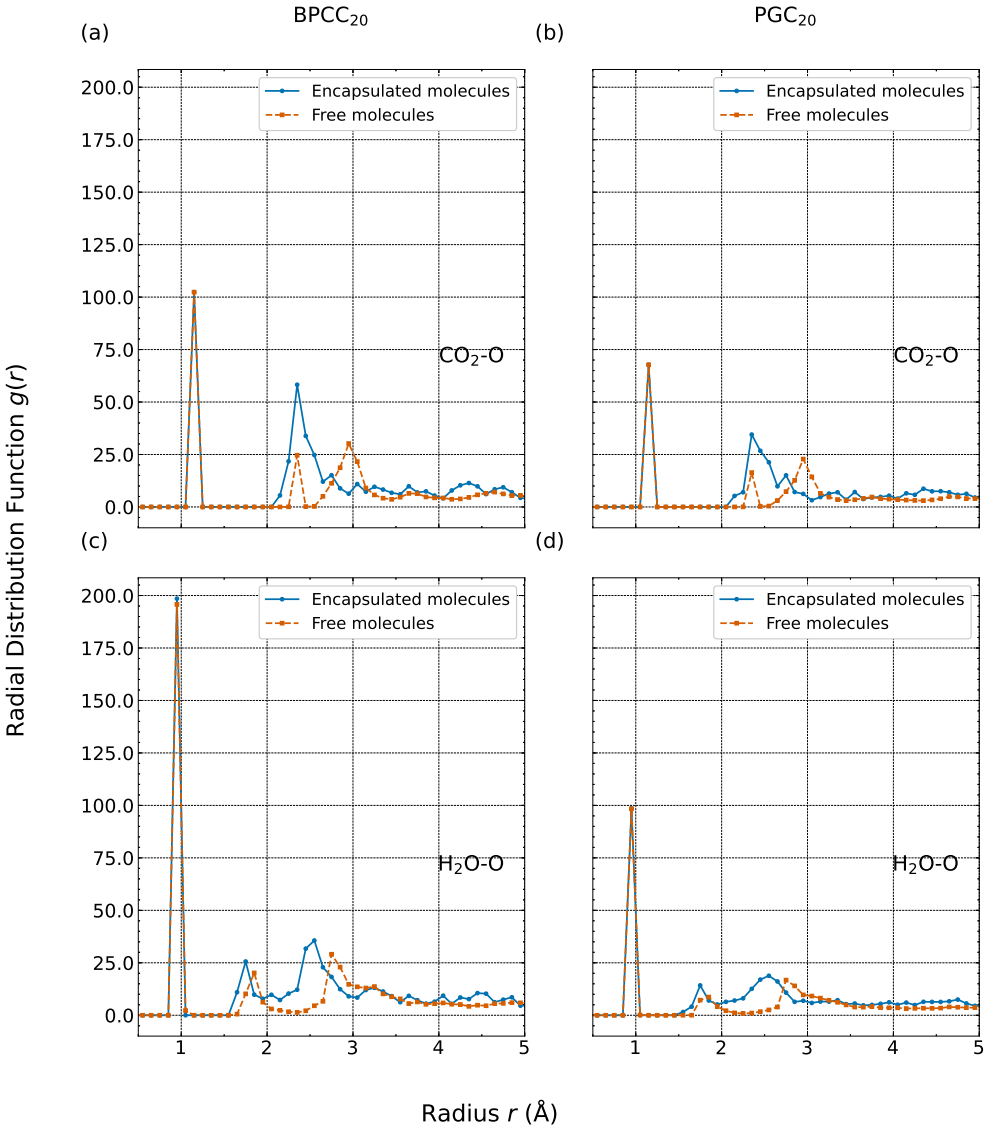



**Fig. 10**: Radial distribution in maximum systems for the distances between $CO_2$ and oxygen atom in (a) $BPCC_{20}$ and (b) $PGC_{20}$, and distances between $H_2O$ and oxygen atom in (c) $BPCC_{20}$ and (d) $PGC_{20}$.

Figure 11 shows the influence of the presence of water molecules close to the endohedral system on the electrostatic potential distribution. One molecule was added per pore around the structures, resulting in the adsorption of these molecules.

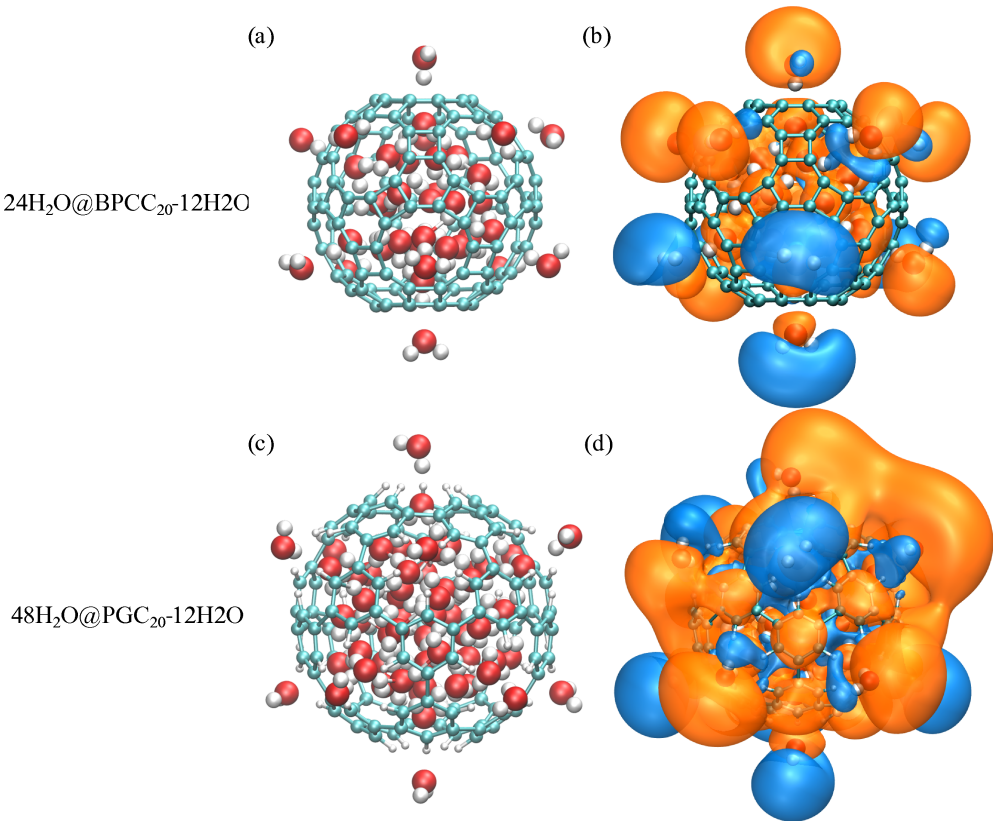



**Fig. 11**: Electrostatic Potential Isosurfaces for maximum capacity systems with $H_2O$ molecules, modified by the external adsorption of molecules of the same species in each pore of the cage structure. (a) $24H_2O@BPCC_{20}$-$12H_2O$ and (b) $48H_2O@PGC_{20}$-$12H_2O$. In both cases, the orange surface represents the negative potential and the blue surface the positive potential. ISO values range from -0.3 to 0.3 for $BPCC_{20}$ and -0.5 to 0.5 for $PGC_{20}$.