Supplementary Information

Molecular Dynamics Study of the Role of Water in the Carbon Dioxide Intercalation in Chloride Ions Bearing Hydrotalcite

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CANADA T6G 1H9

1. Atomic Density Profile

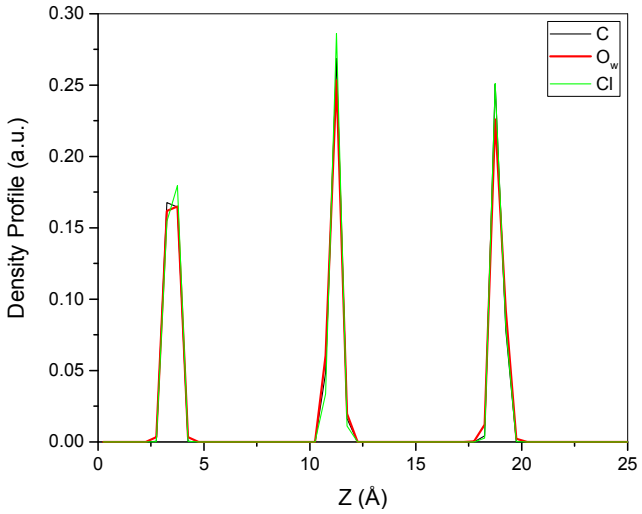


Figure S 1-Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 36 CO_2 and 36 H_2O.

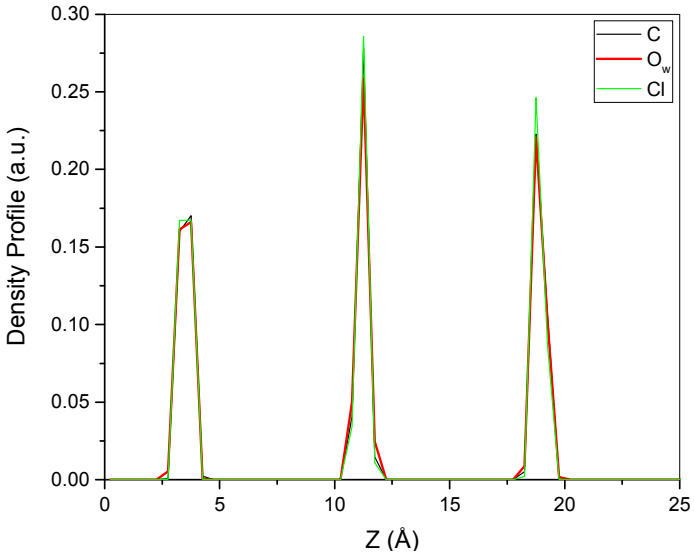


Figure S 2-Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 84 CO_2 and 36 H_2O.

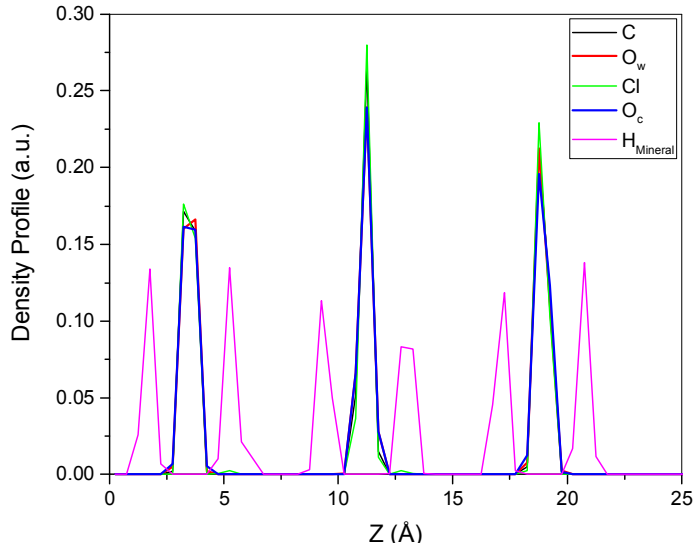


Figure S 3- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 120 CO_2 and 36 H_2O.

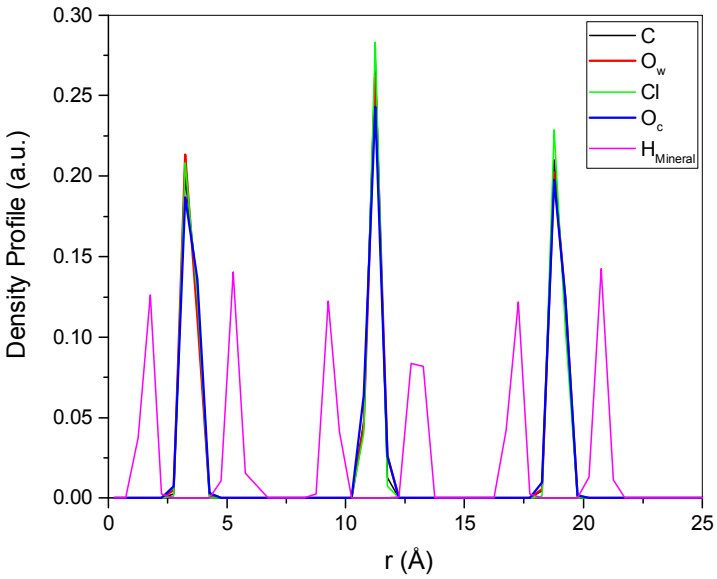


Figure S 4- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 216 CO_2 and 36 H_2O.

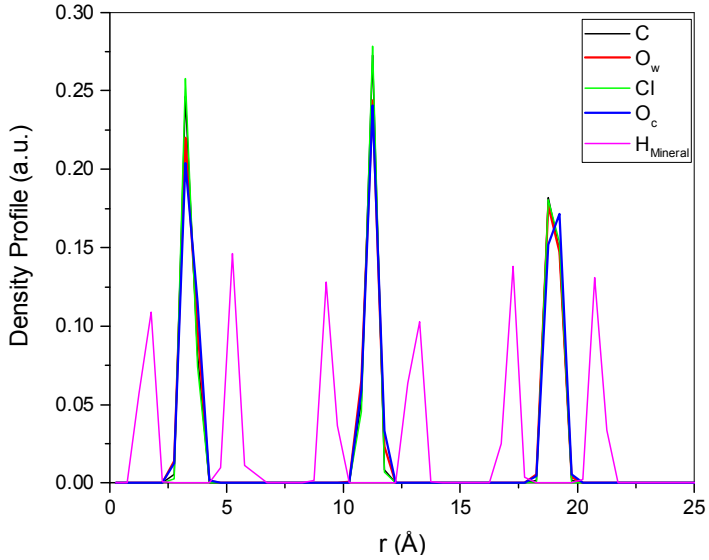


Figure S 5- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 432 CO_2 and 36 H_2O.

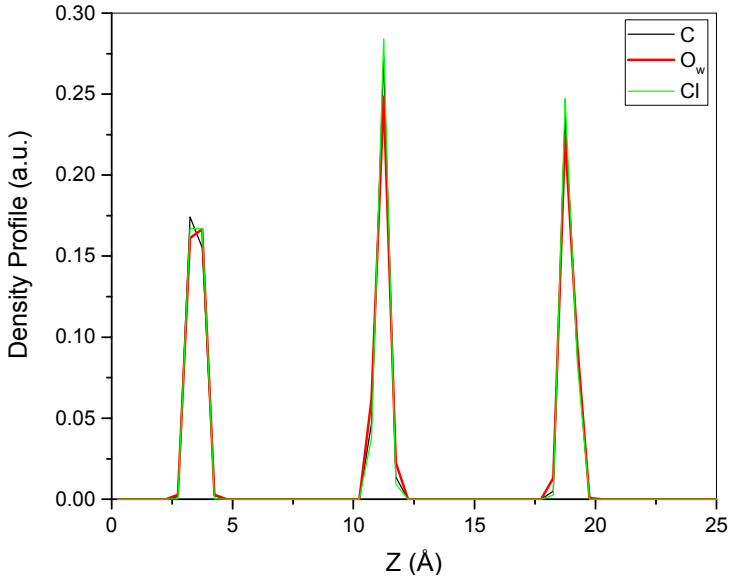


Figure S 6- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 36 CO_2 and 72 H_2O.

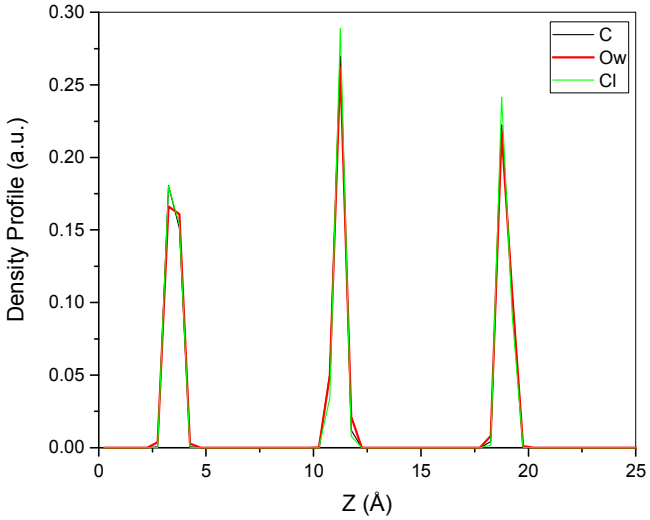


Figure S 7- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 84 CO_2 and 72 H_2O.

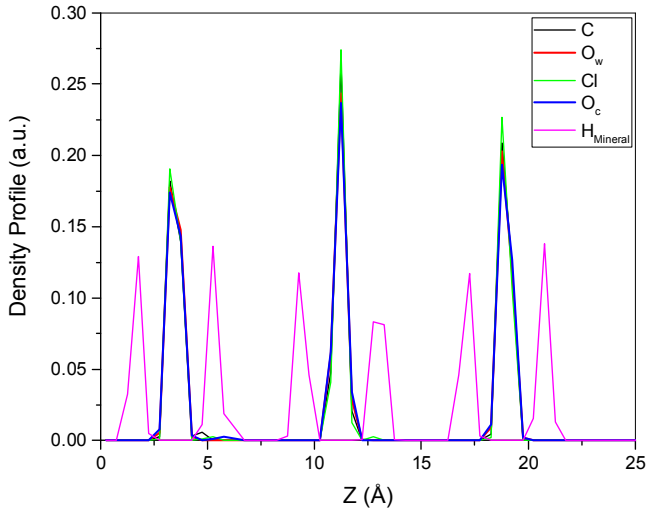


Figure S 8- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 120 CO_2 and 72 H_2O.

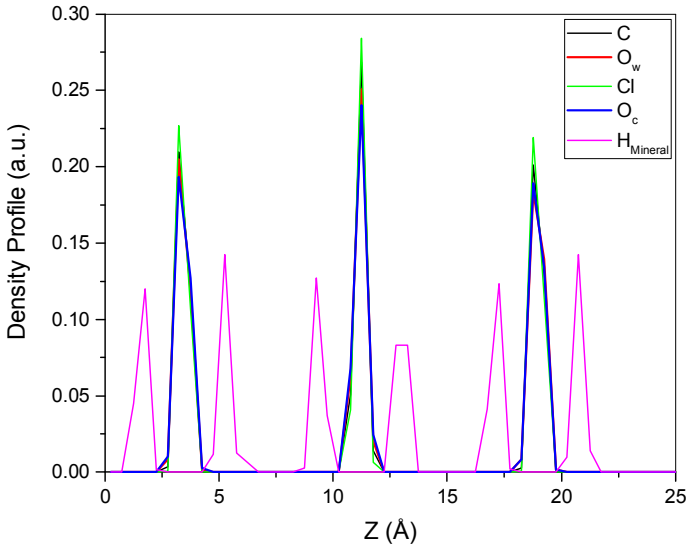


Figure S 9- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 216 CO_2 and 72 H_2O.

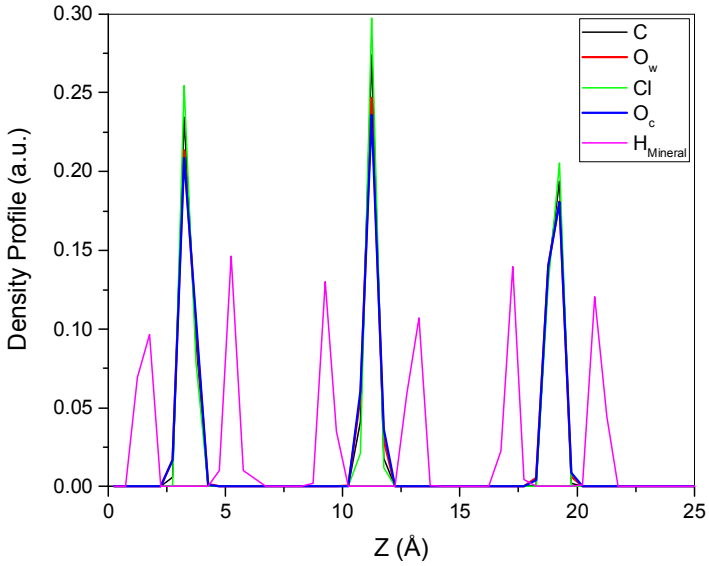


Figure S 10- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 432 CO_2 and 72 H_2O.

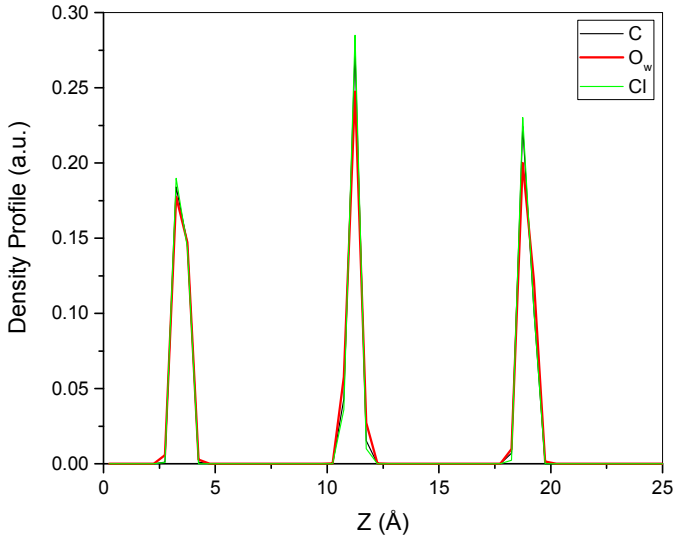


Figure S 11- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 36 CO_2 and 144 H_2O.

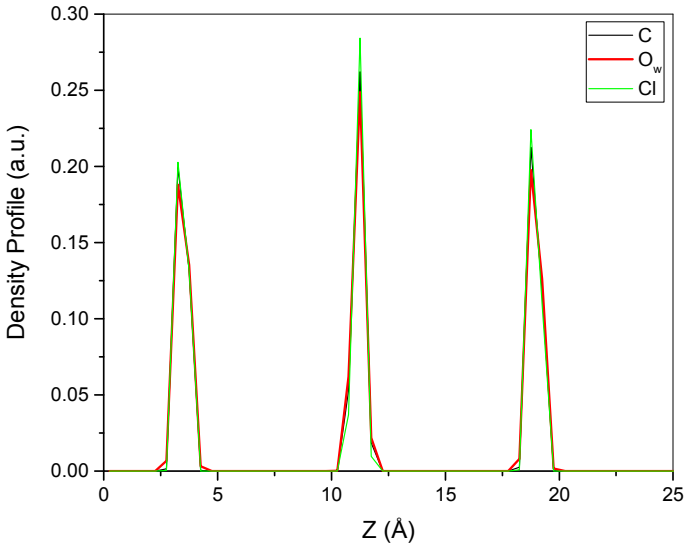


Figure S 12- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 84 CO_2 and 144 H_2O.

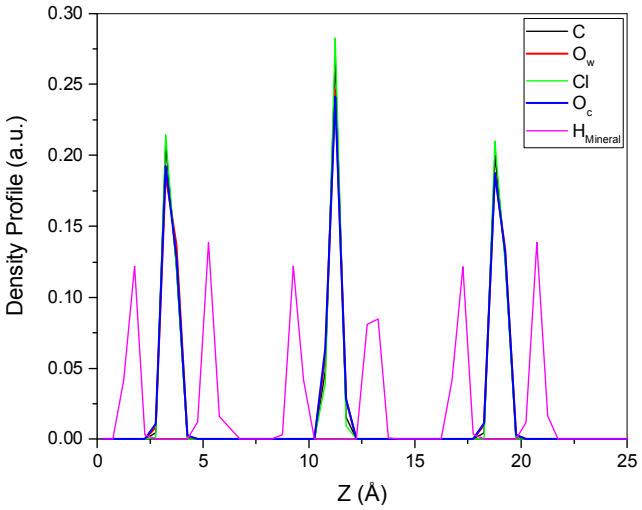


Figure S 13- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 120 CO_2 and 144 H_2O.

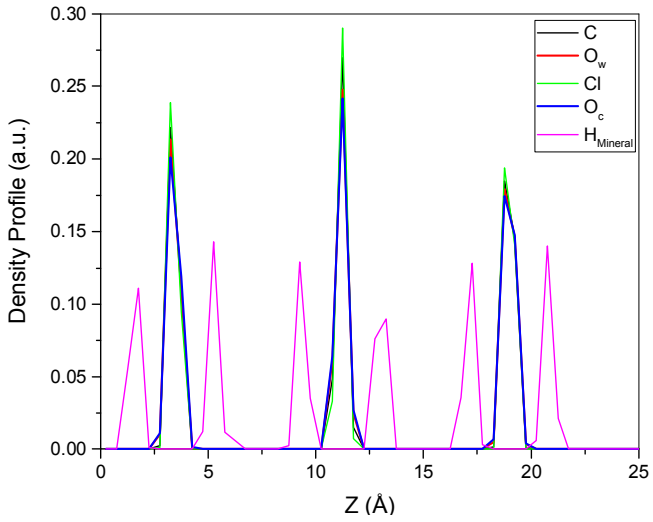


Figure S 14- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 216 CO_2 and 144 H_2O.

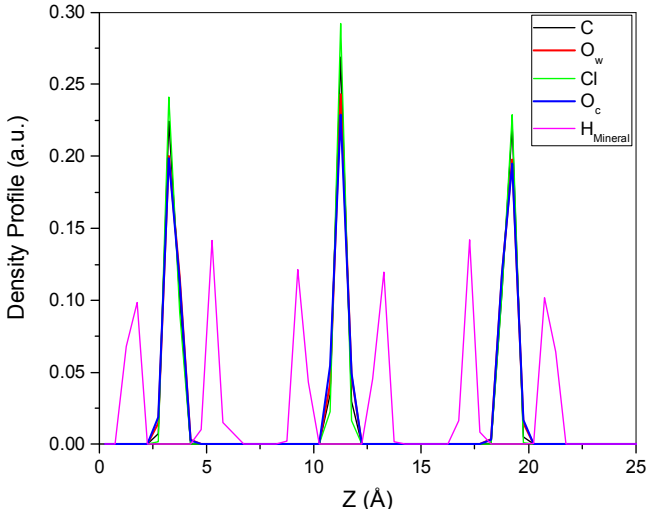


Figure S 15- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 432 CO_2 and 144 H_2O.

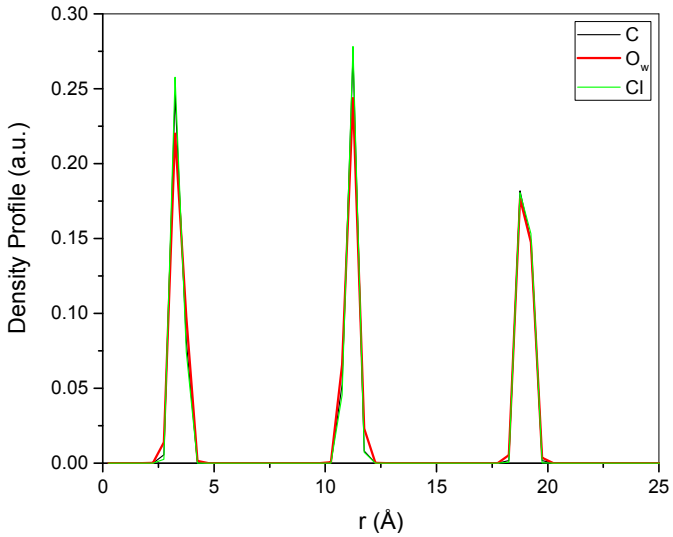


Figure S 16- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 36 CO_2 and 432 H_2O.

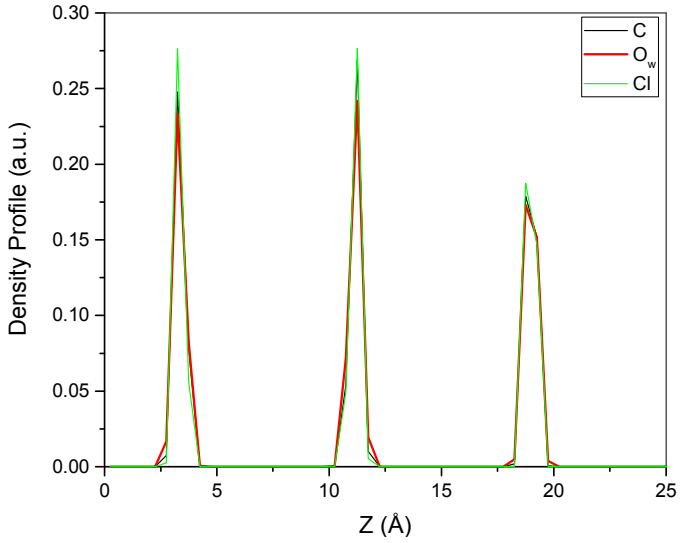


Figure S 17- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 84 CO_2 and 432 H_2O.

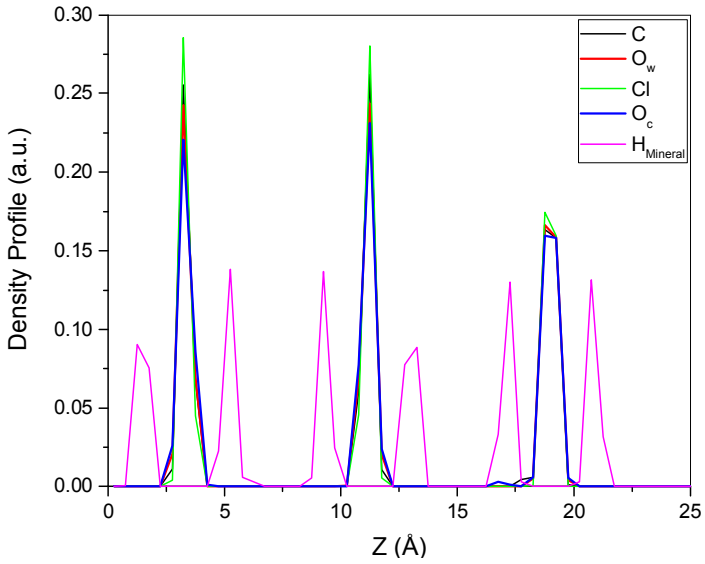


Figure S 18- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 120 CO_2 and 432 H_2O.

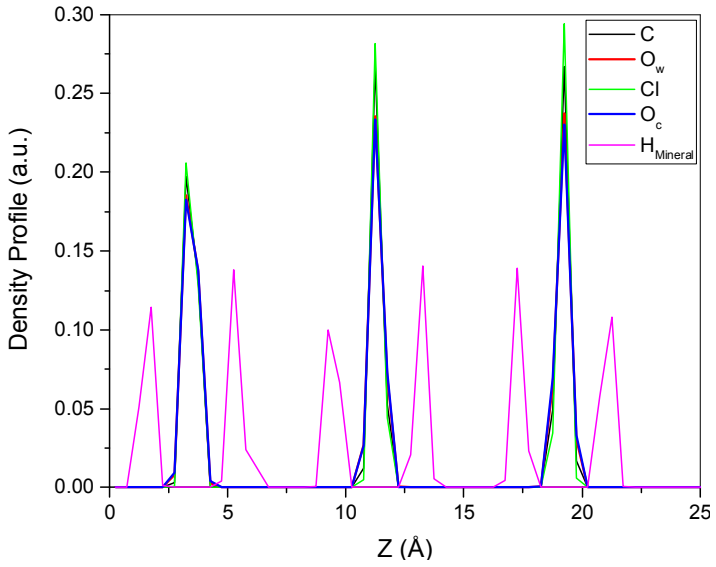


Figure S 19- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 216 CO_2 and 432 H_2O.

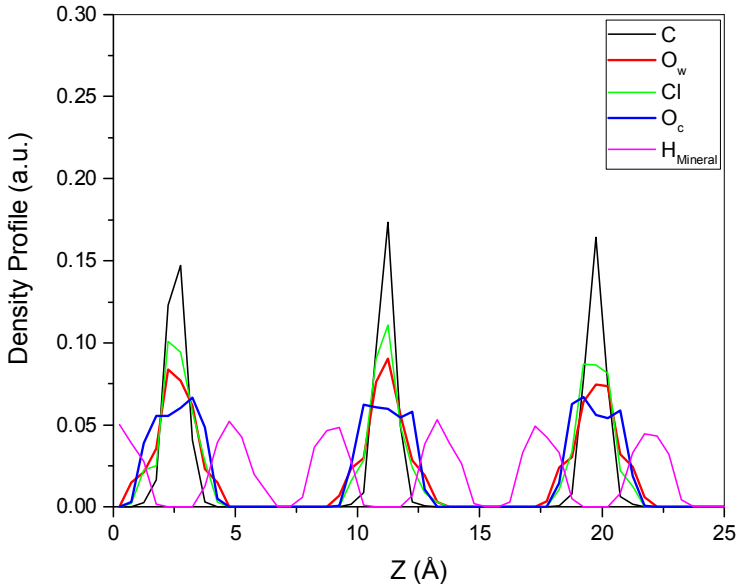


Figure S 20- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 432 CO_2 and 432 H_2O.

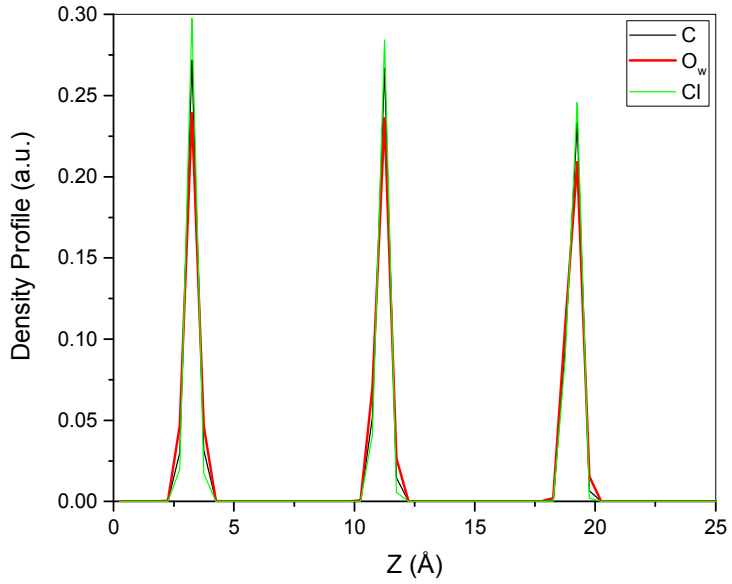


Figure S 21- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 36 CO_2 and 864 H_2O.

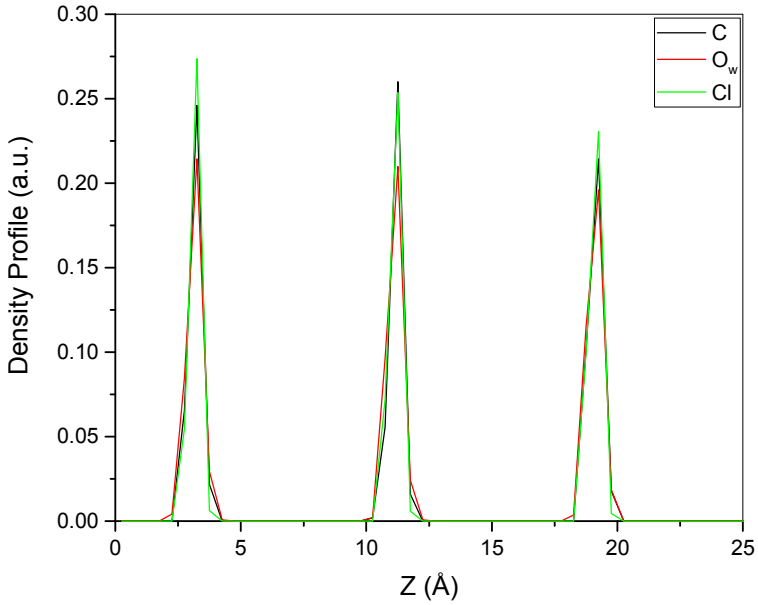


Figure S 22- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 84 CO_2 and 864 H_2O.

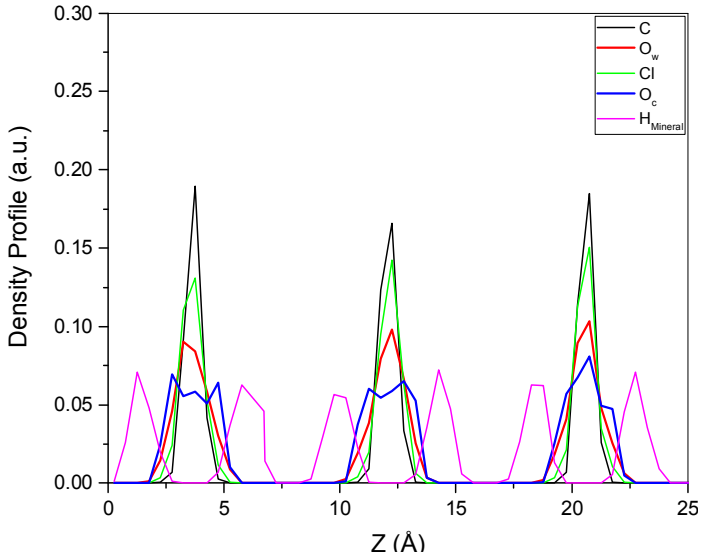


Figure S 23- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 216 CO_2 and 864 H_2O.

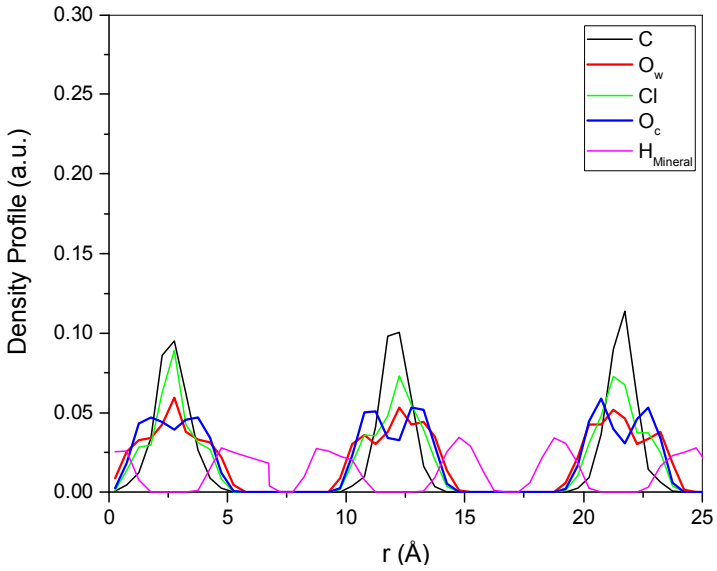
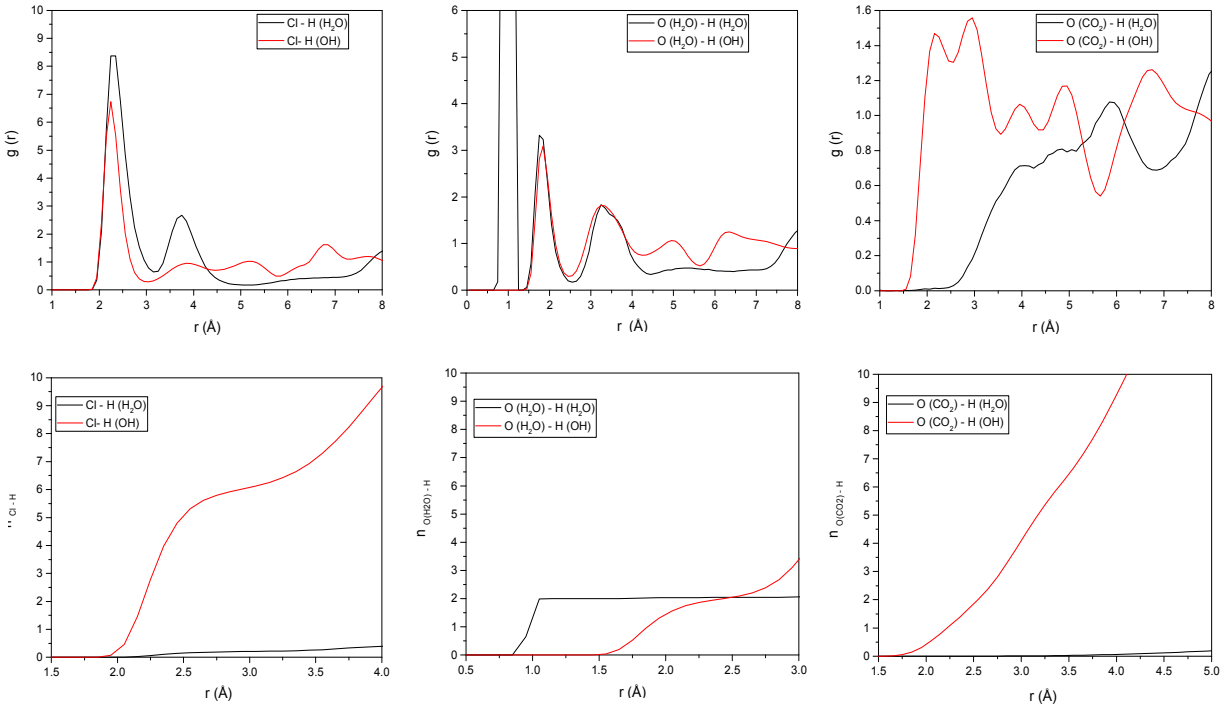


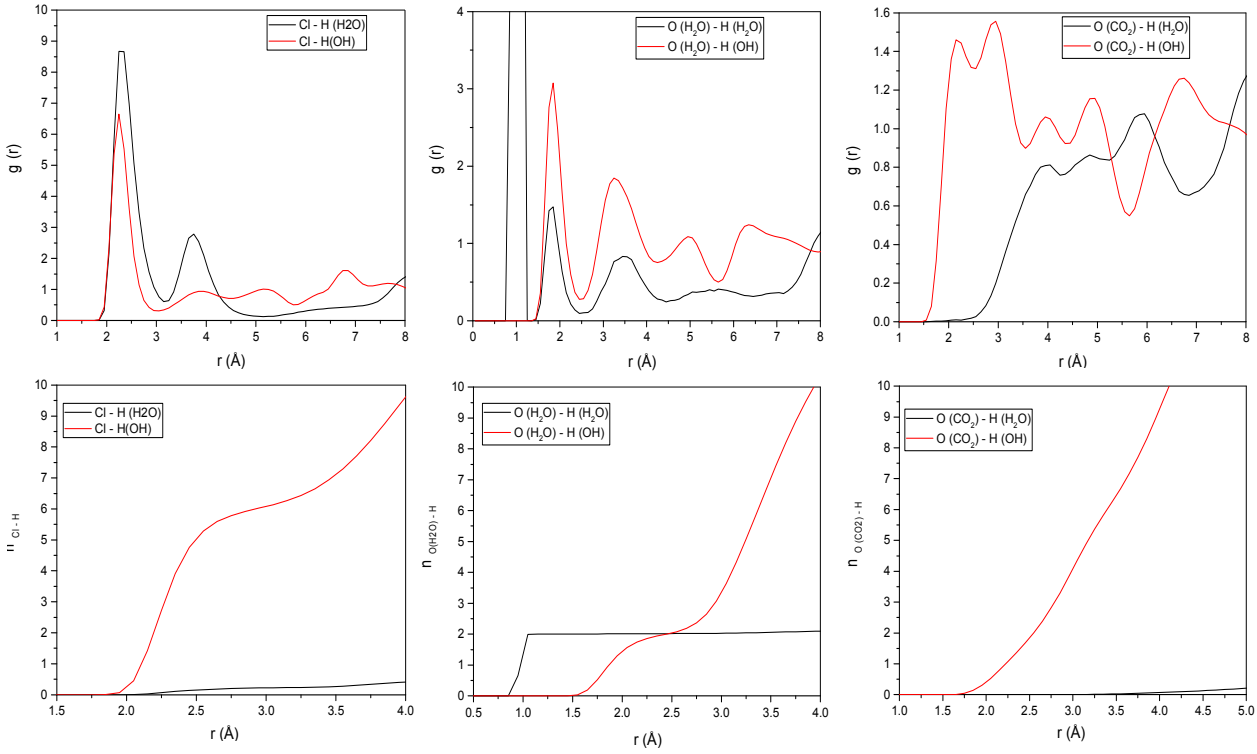
Figure S 24- Atomic density profiles of interlayer H_2O and CO_2 in the simulation cell along the z dimension (perpendicular to the mineral surface) for the system containing 432 CO_2 and 864 H_2O.

2. Hydrogen Bonds Calculations



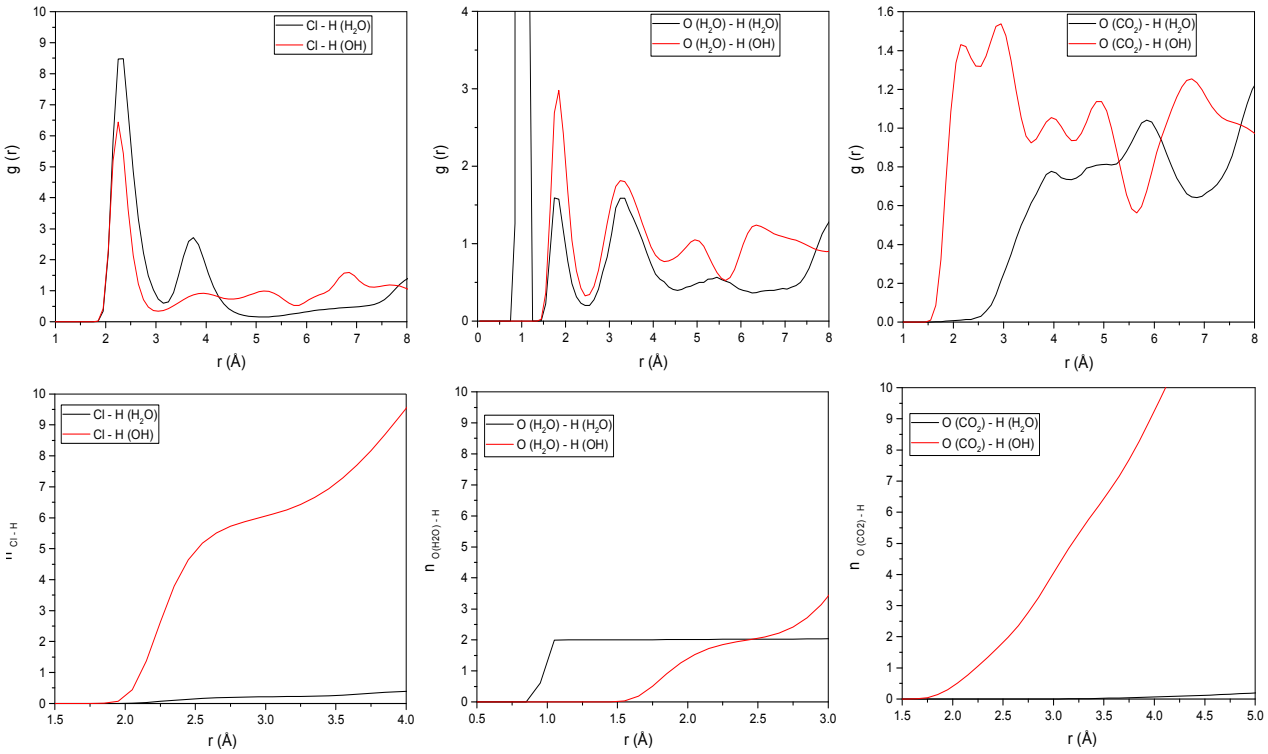
An average number of hydrogen bonds per interlayer water molecule = 1.2

Figure S 25- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 36 CO_2 and 36 H_2O in the interlayer region.



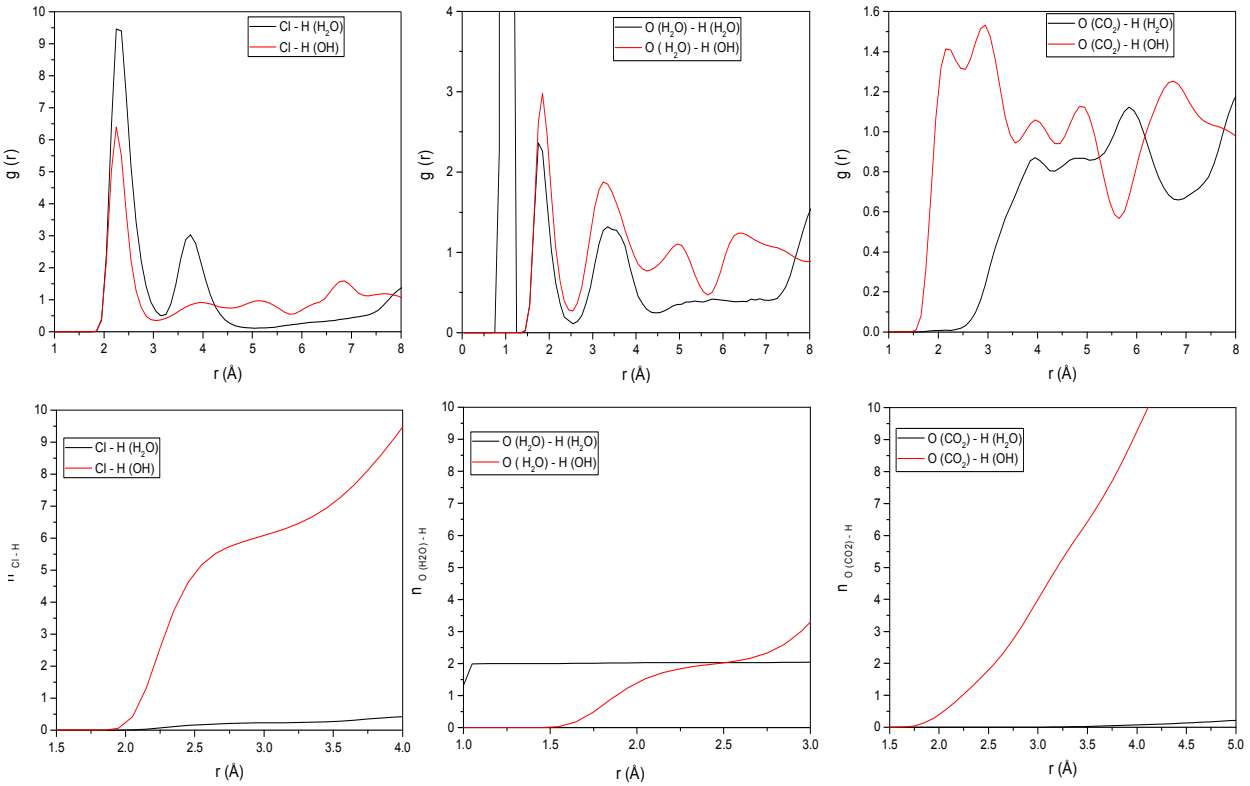
An average number of hydrogen bonds per interlayer water molecule = 1.2

Figure S 26- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 84 CO_2 and 36 H_2O in the interlayer region.



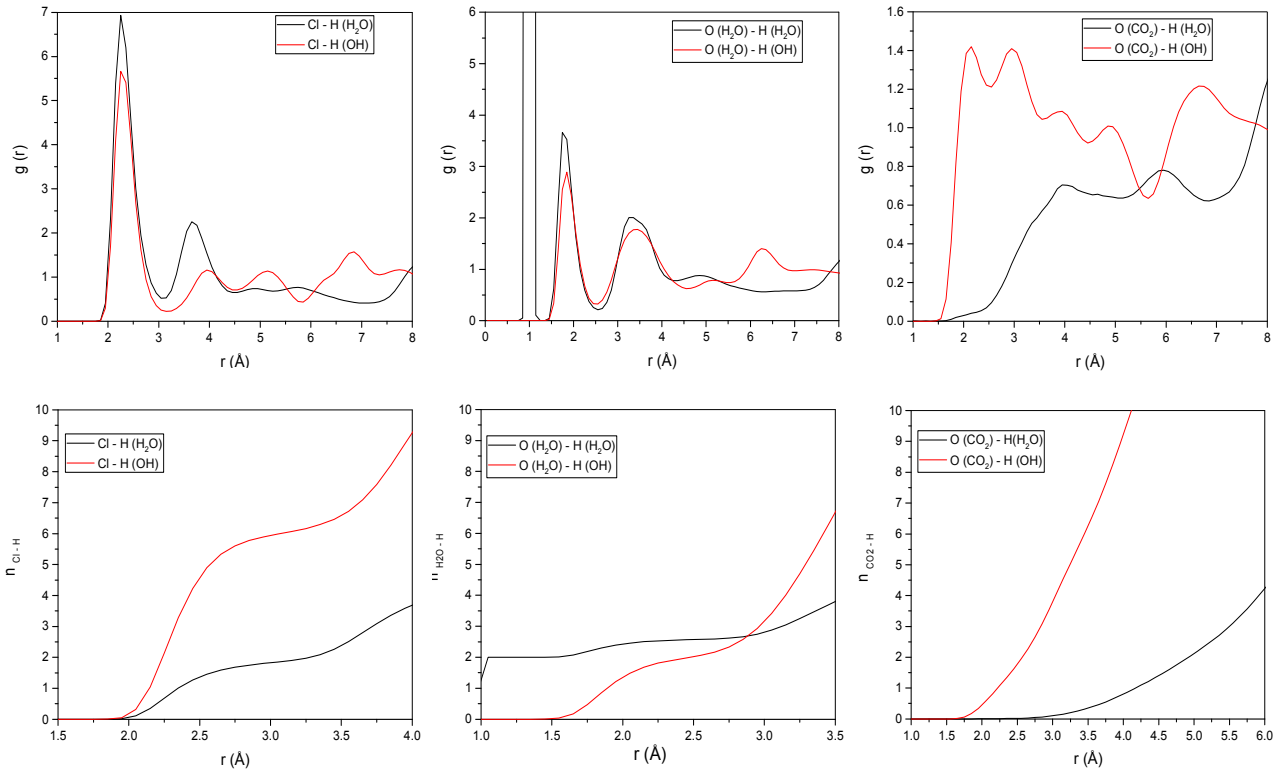
An average number of hydrogen bonds per interlayer water molecule = 1.2

Figure S 27- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 120 CO_2 and 36 H_2O in the interlayer region.



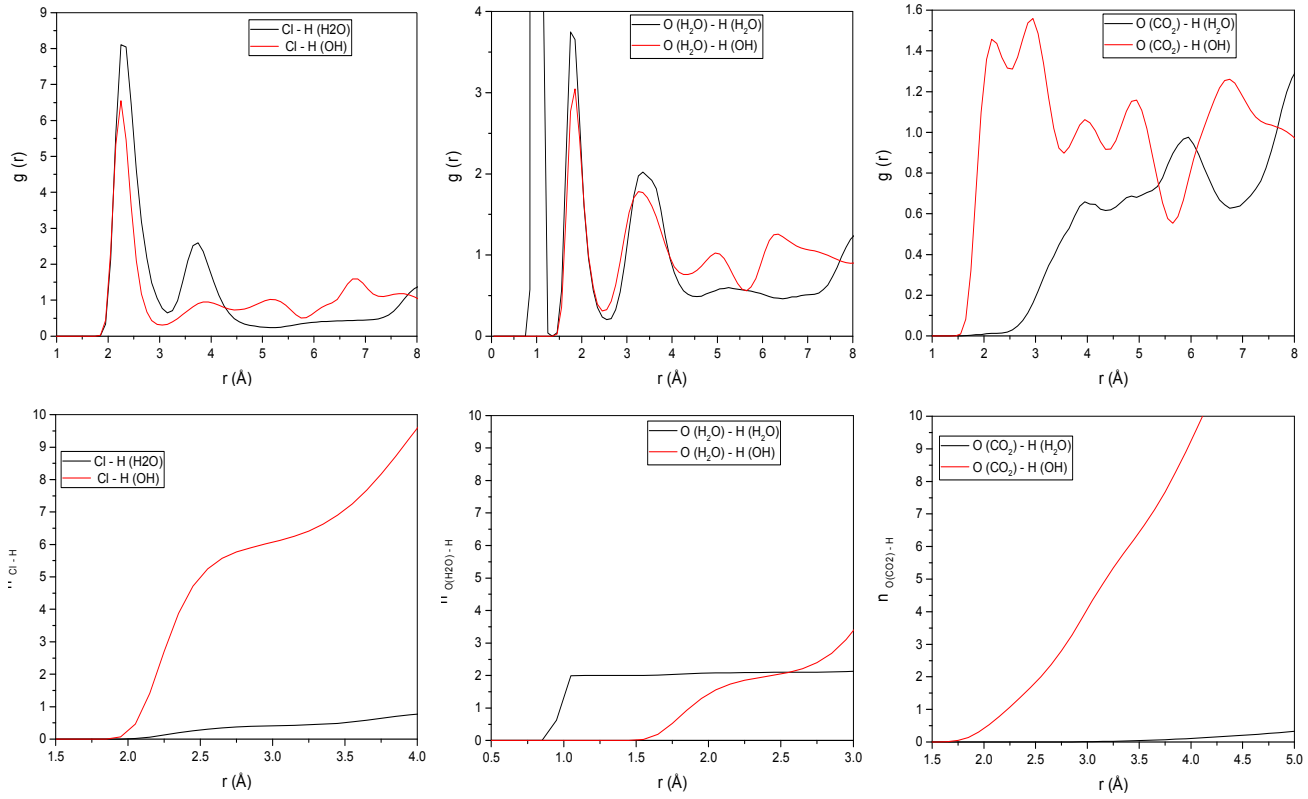
An average number of hydrogen bonds per interlayer water molecule = 1.2

Figure S 28- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 216 CO_2 and 36 H_2O in the interlayer region.



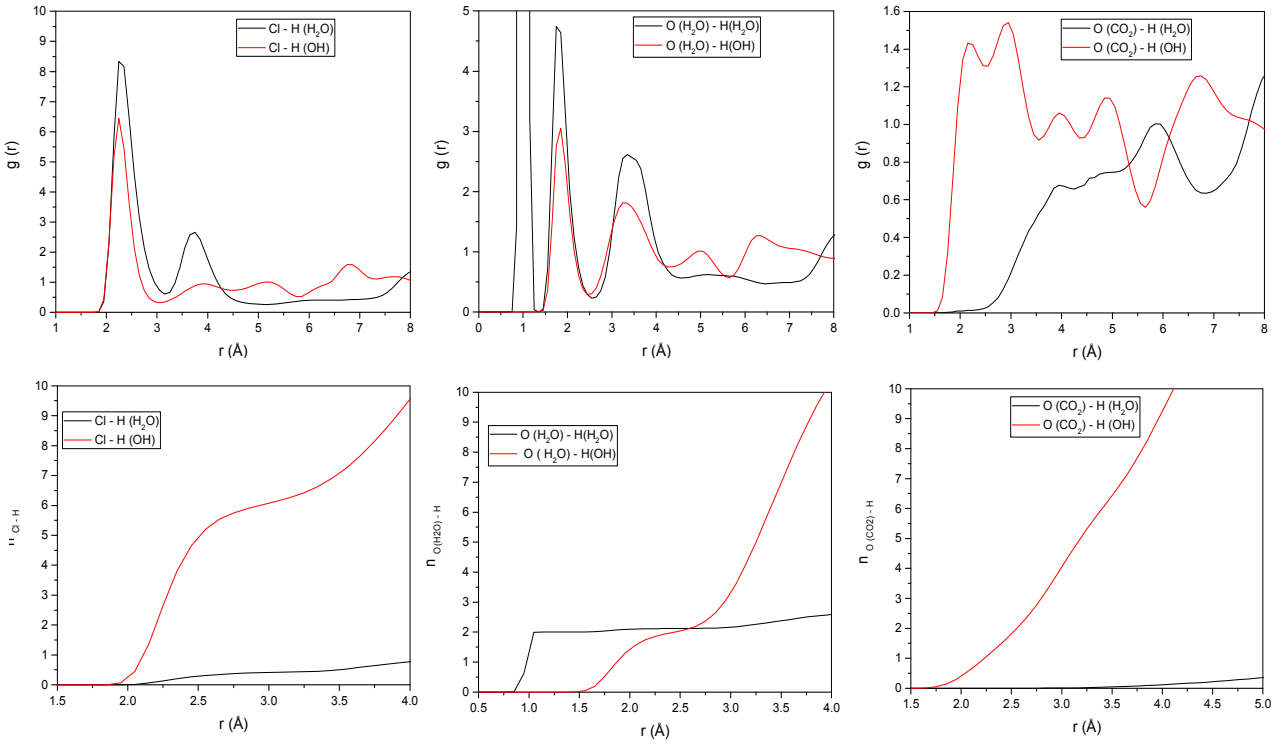
An average number of hydrogen bonds per interlayer water molecule = 1.27

Figure S 29- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 432 CO_2 and 36 H_2O in the interlayer region.



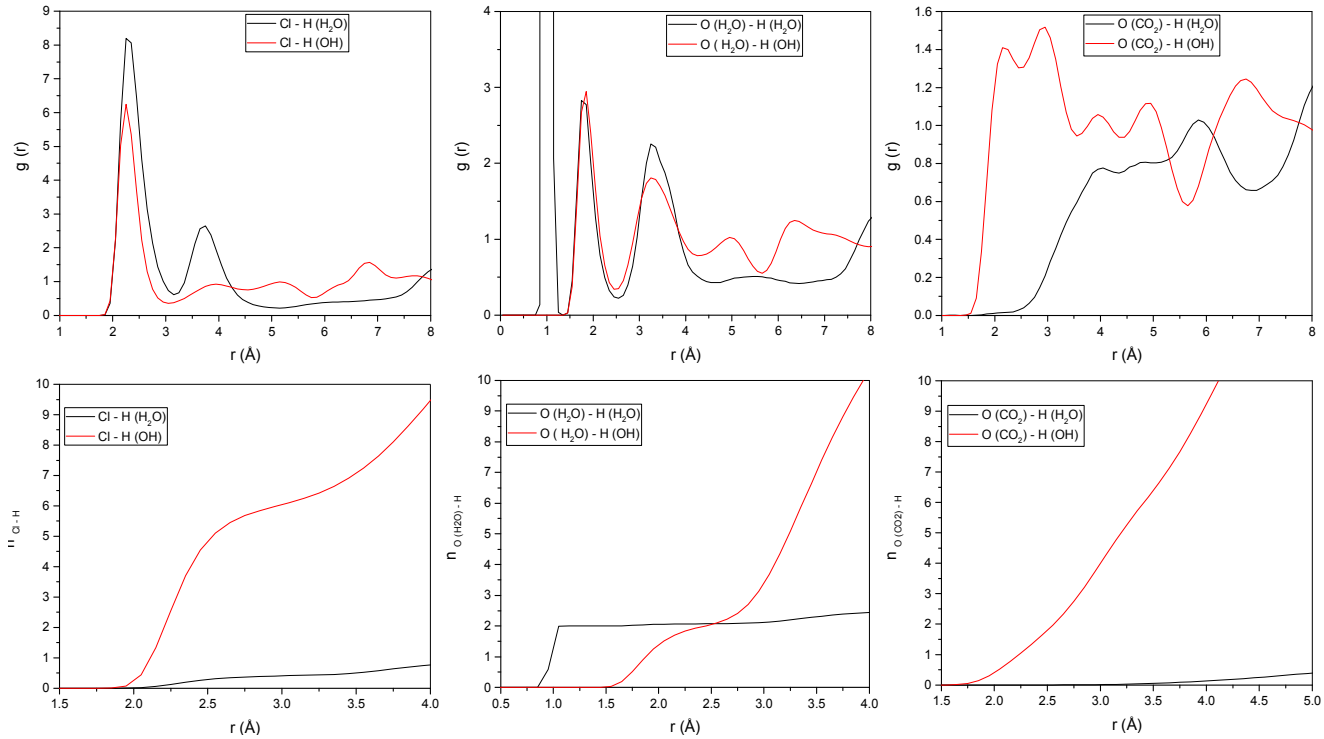
An average number of hydrogen bonds per interlayer water molecule = 1.4

Figure S 30- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 36 CO_2 and 72 H_2O in the interlayer region.



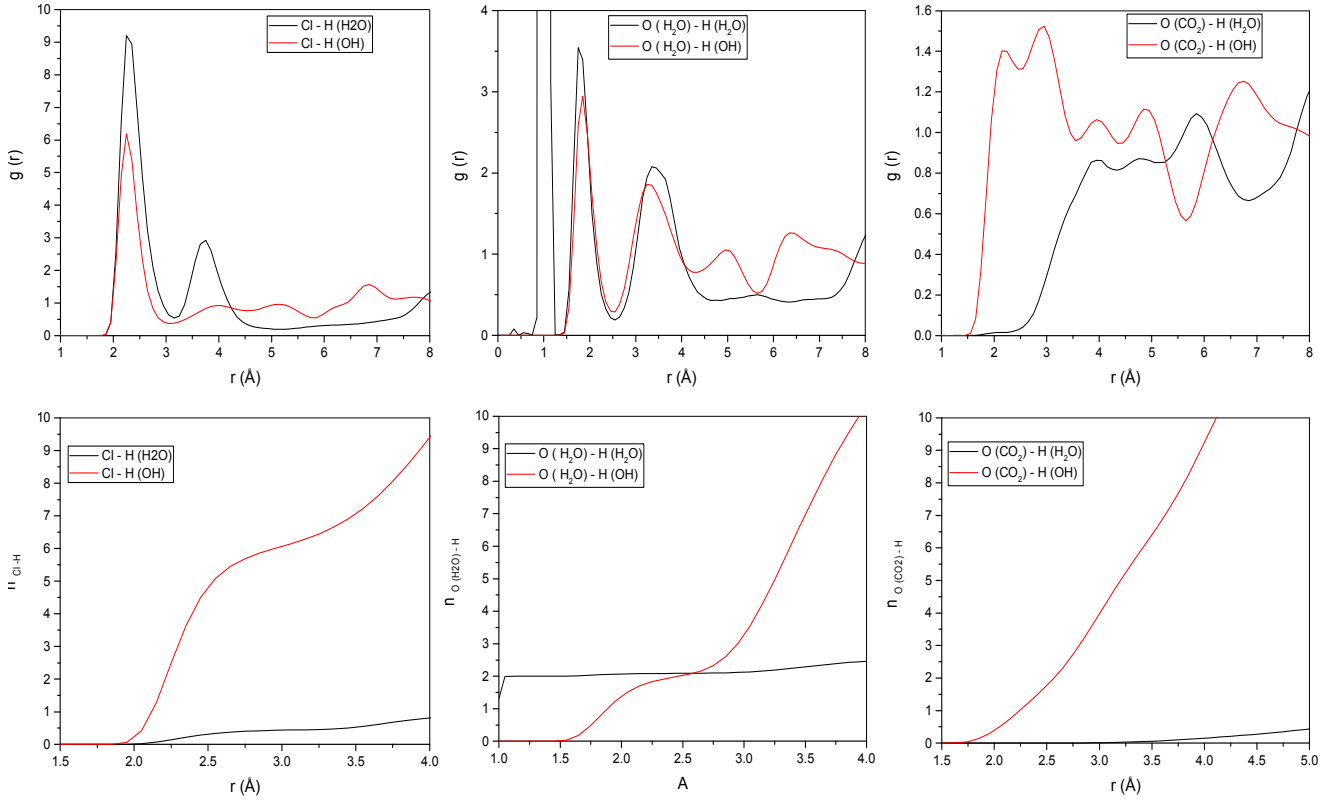
An average number of hydrogen bonds per interlayer water molecule = 1.47

Figure S 31- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 84 CO_2 and 72 H_2O in the interlayer region.



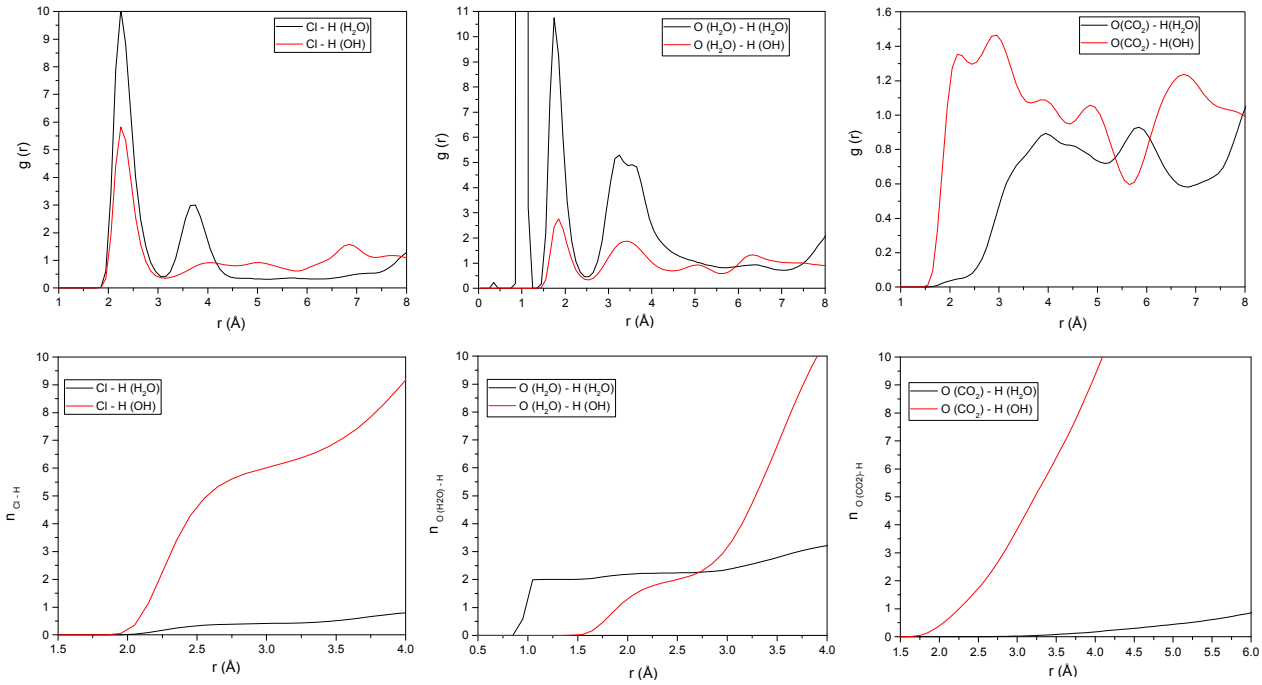
An average number of hydrogen bonds per interlayer water molecule = 1.55

Figure S 32- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 120 CO_2 and 72 H_2O in the interlayer region.



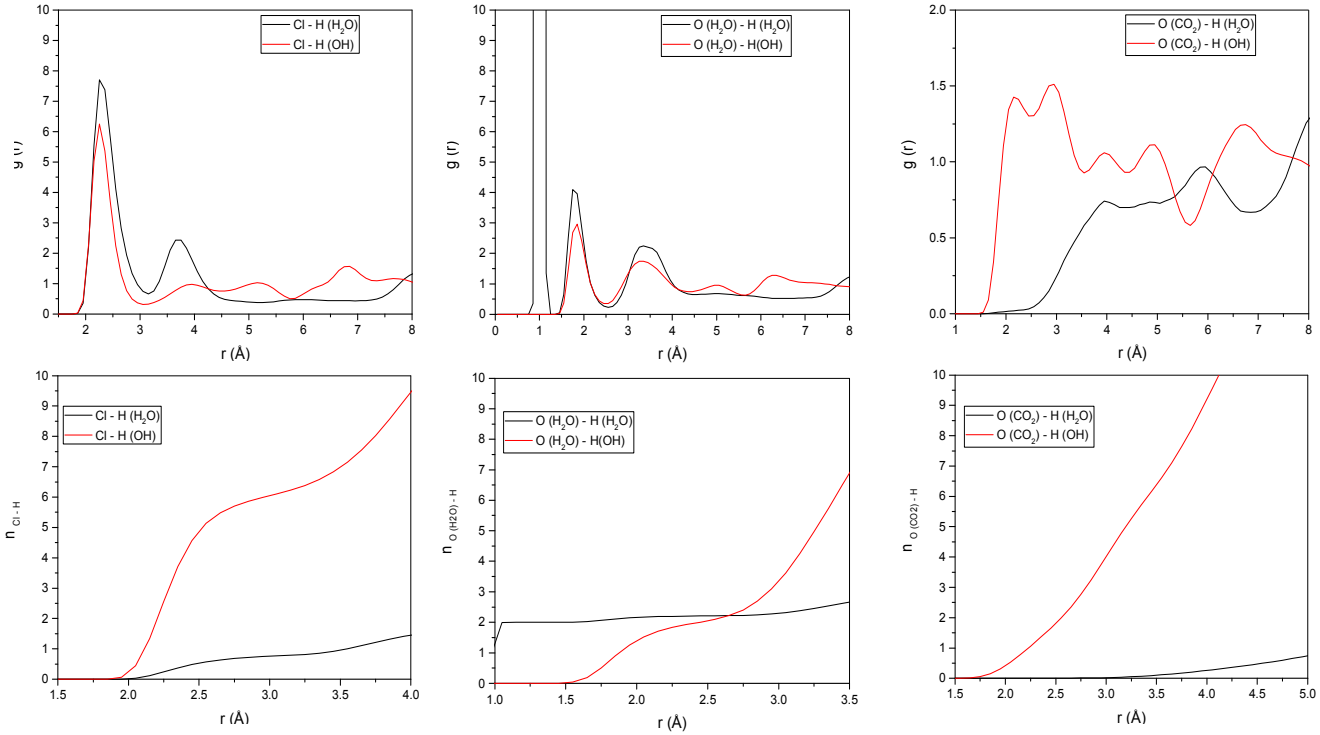
An average number of hydrogen bonds per interlayer water molecule = 1.55

Figure S 33- Pair Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 216 CO_2 and 72 H_2O in the interlayer region.



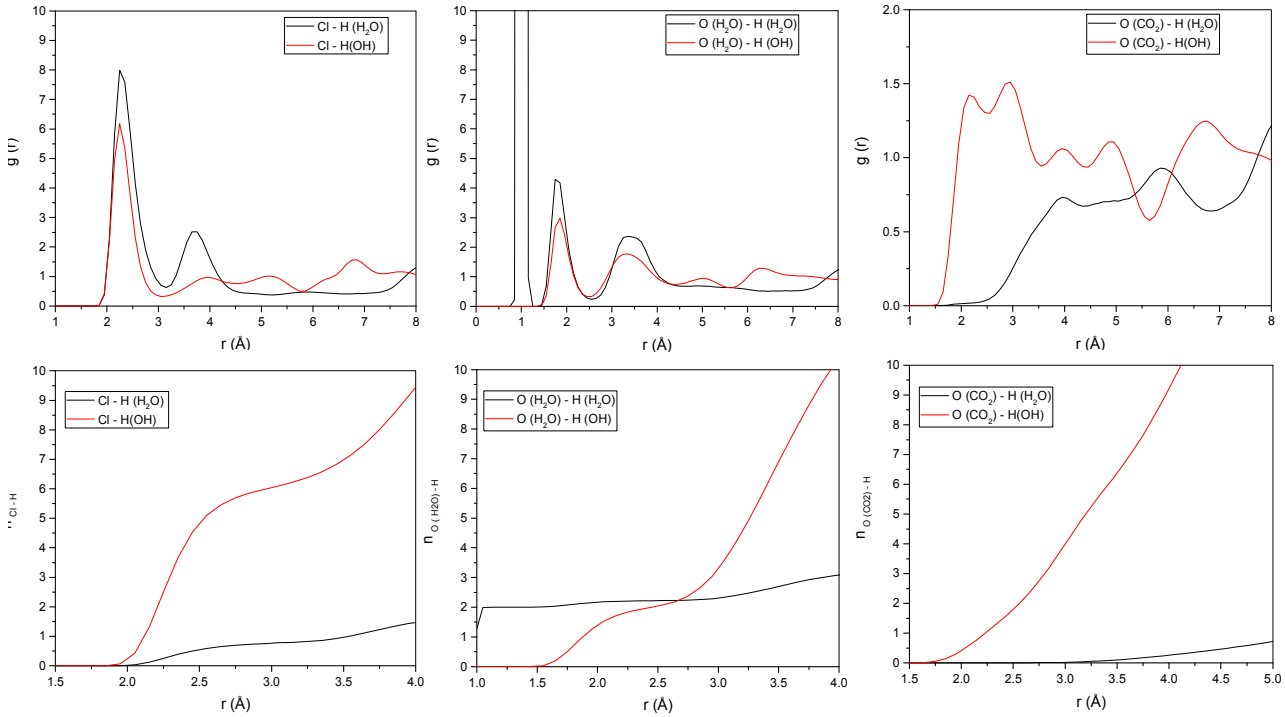
An average number of hydrogen bonds per interlayer water molecule = 1.75

Figure S 34- Pair Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 432 CO_2 and 72 H_2O in the interlayer region.



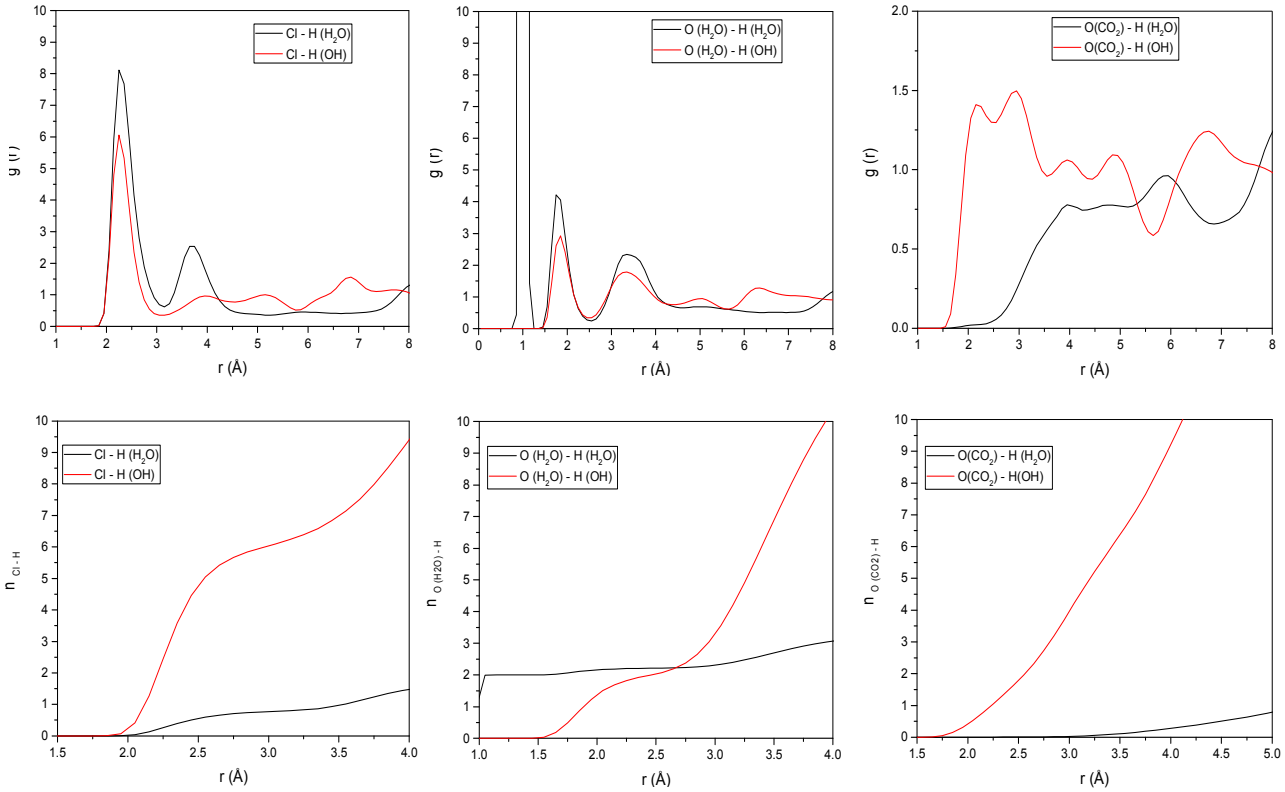
An average number of hydrogen bonds per interlayer water molecule = 2.75

Figure S 35- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 36 CO_2 and 144 H_2O in the interlayer region.



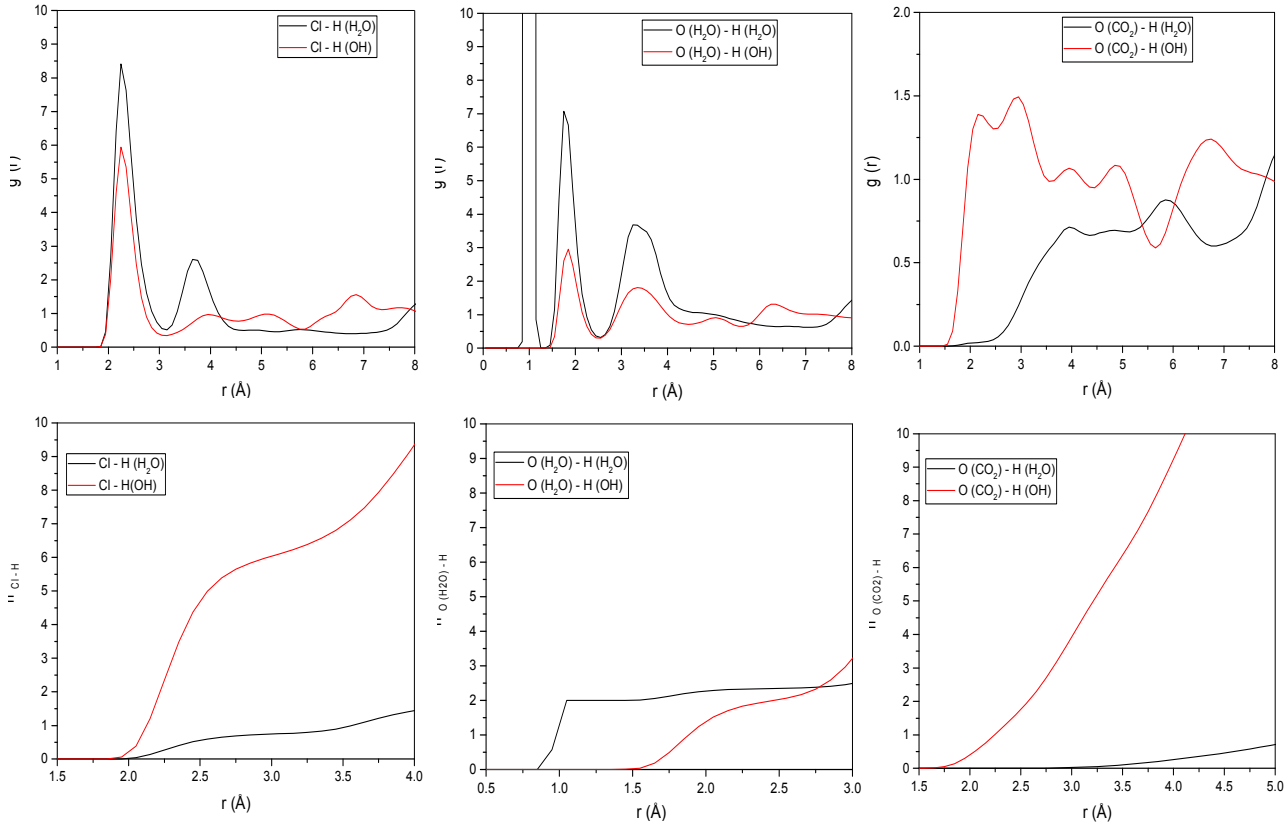
An average number of hydrogen bonds per interlayer water molecule = 2.75

Figure S 36- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 84 CO_2 and 144 H_2O in the interlayer region.



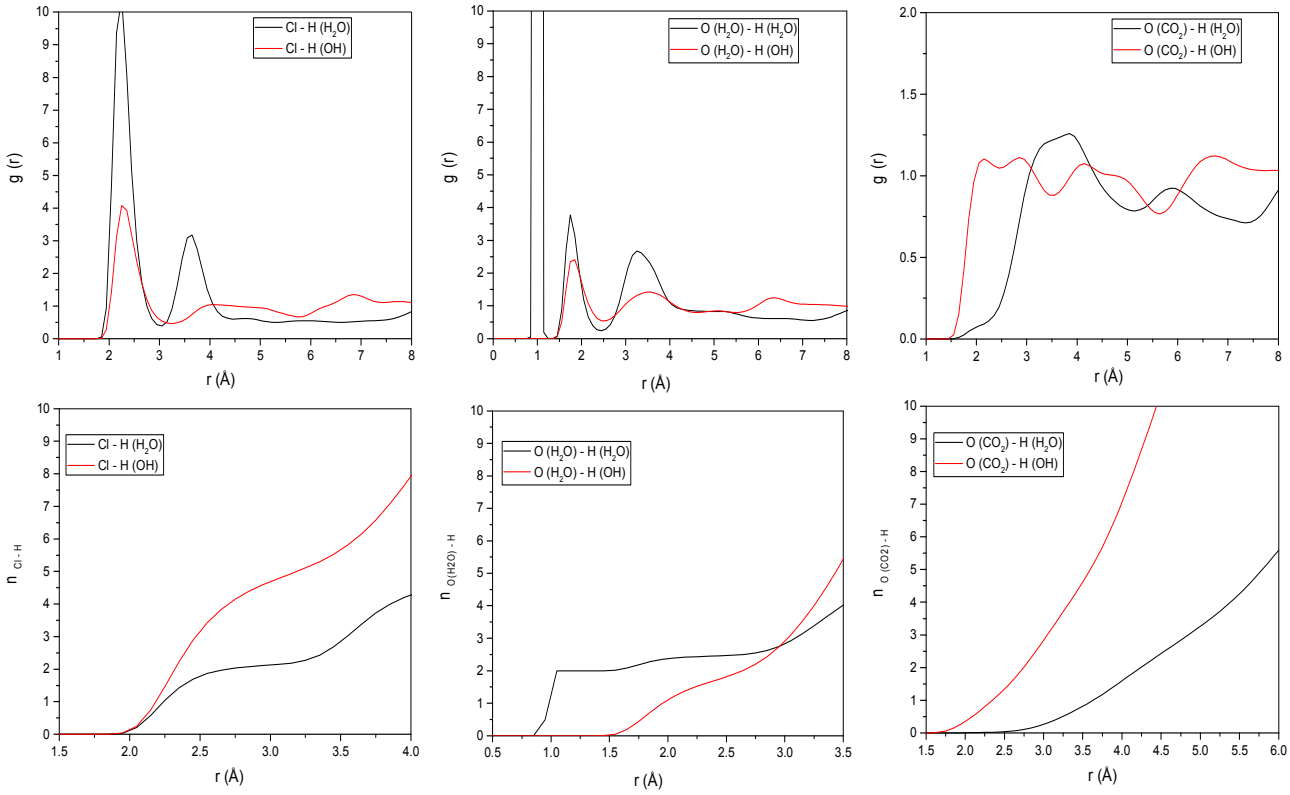
An average number of hydrogen bonds per interlayer water molecule = 2.75

Figure S 37- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 120 CO_2 and 144 H_2O in the interlayer region.



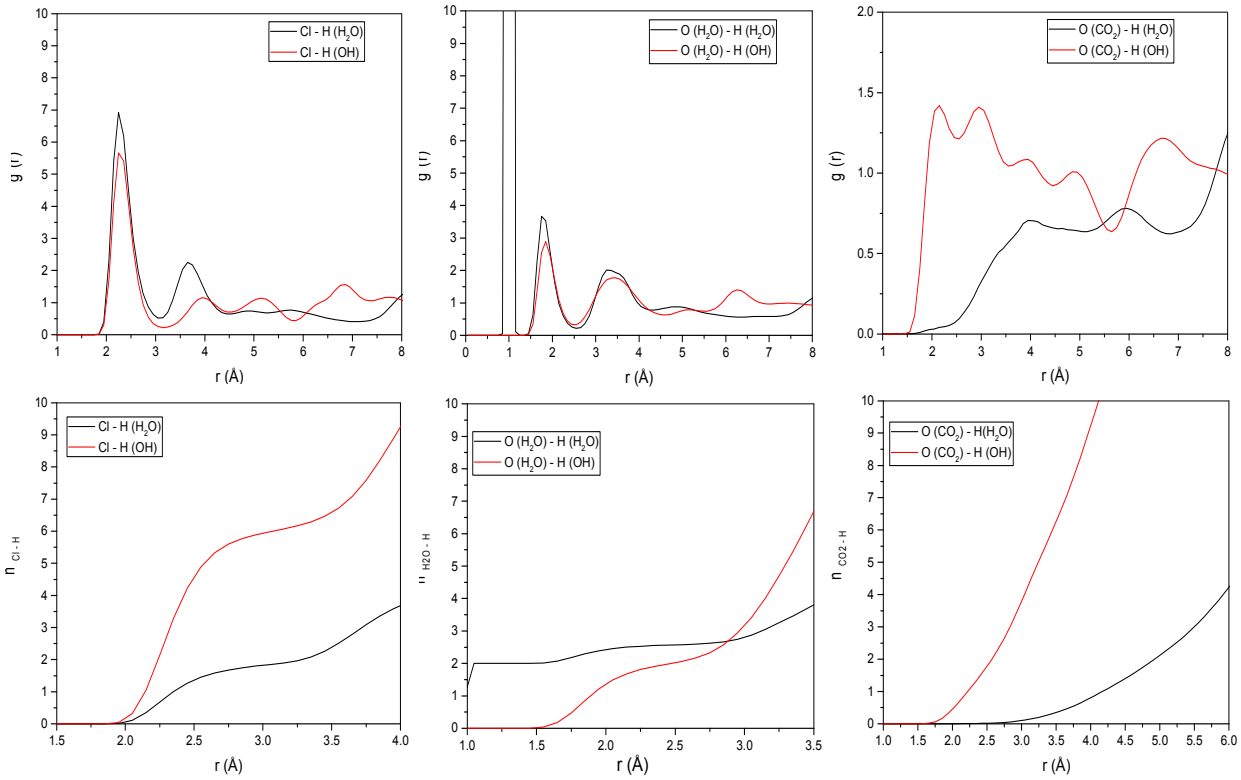
An average number of hydrogen bonds per interlayer water molecule = 2.75

Figure S 38- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 216 CO_2 and 144 H_2O in the interlayer region.



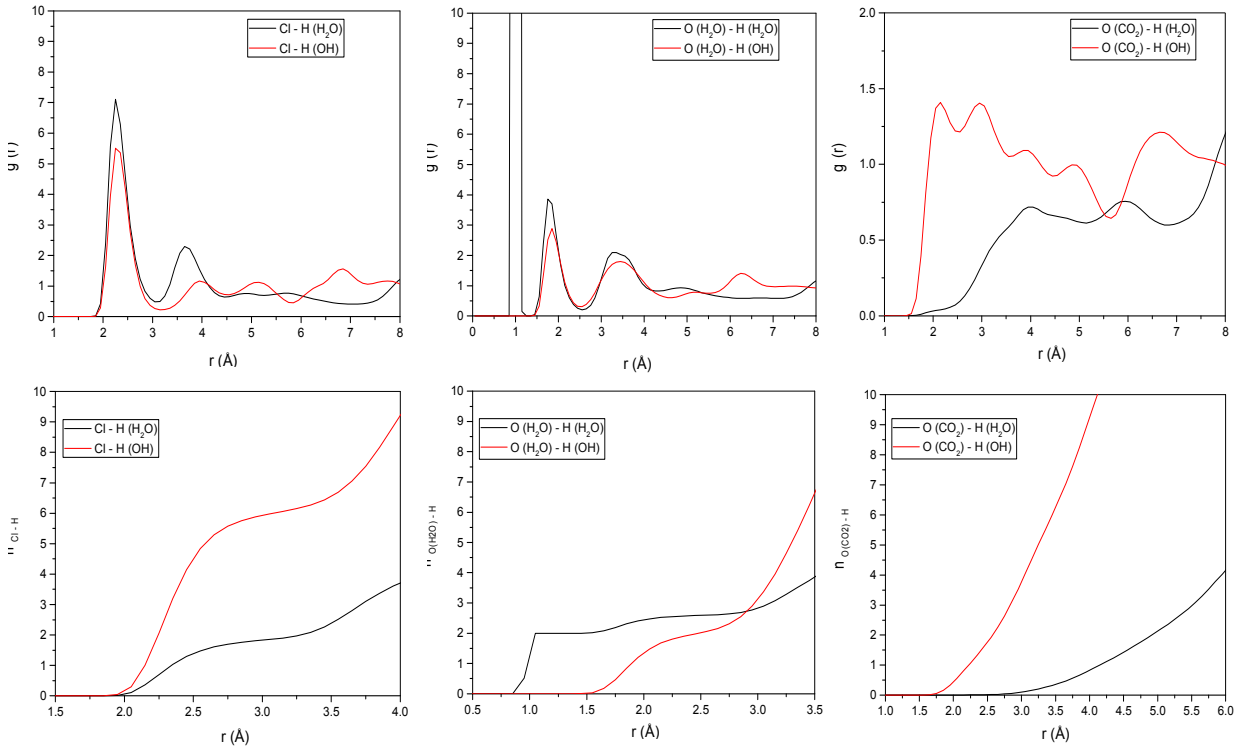
An average number of hydrogen bonds per interlayer water molecule = 2.75

Figure S 39- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 432 CO_2 and 144 H_2O in the interlayer region.



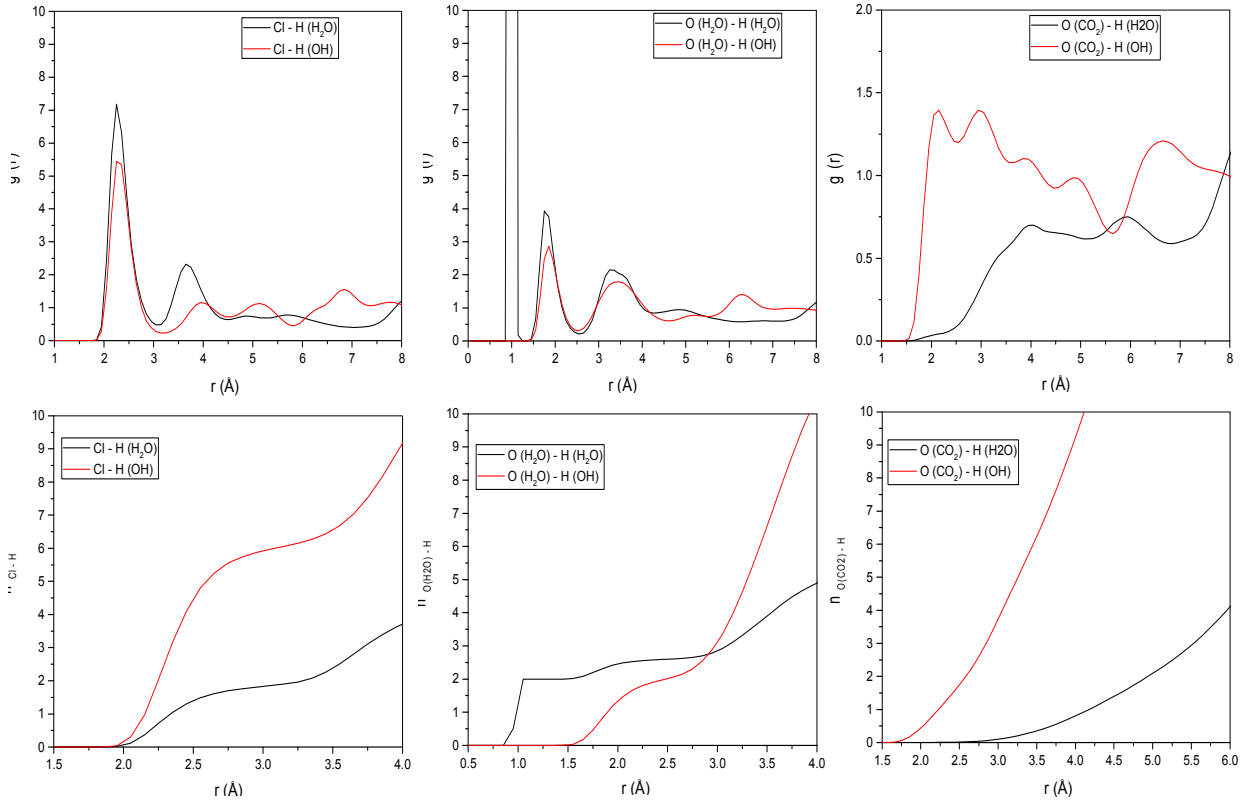
An average number of hydrogen bonds per interlayer water molecule = 3.2

Figure S 40- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 36 CO_2 and 432 H_2O in the interlayer region.



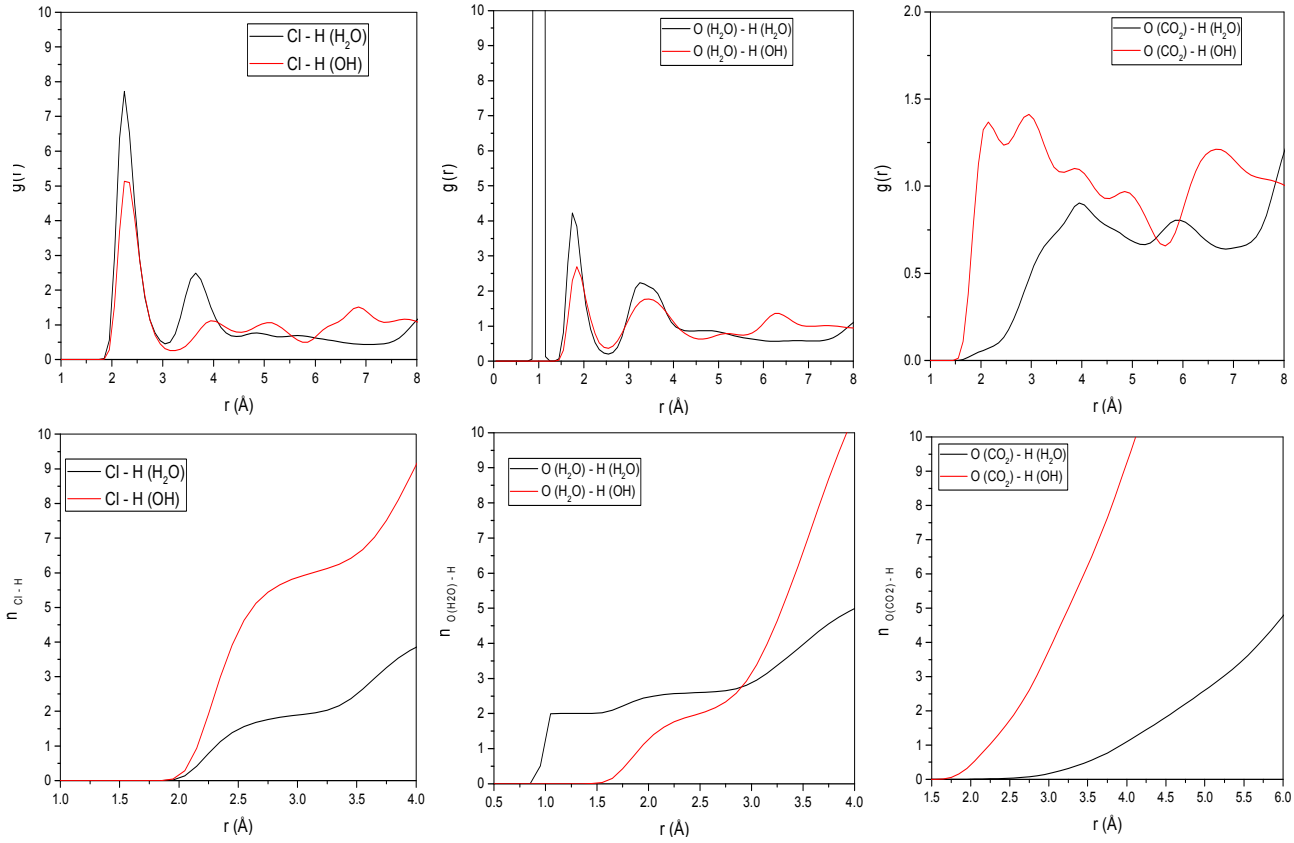
An average number of hydrogen bonds per interlayer water molecule = 3.4

Figure S 41- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 84 CO_2 and 432 H_2O in the interlayer region.



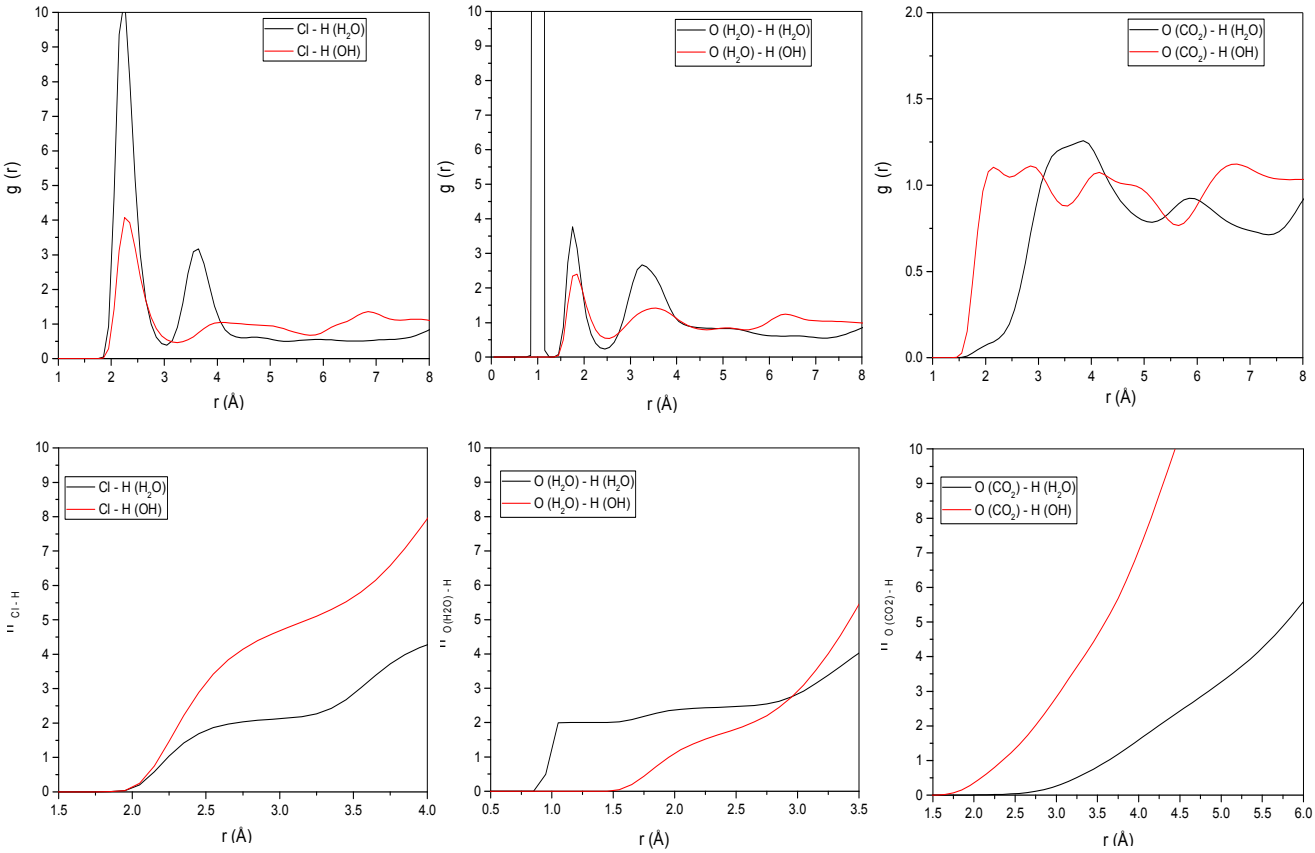
An average number of hydrogen bonds per interlayer water molecule = 3.4

Figure S 42- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 120 CO_2 and 432 H_2O in the interlayer region.



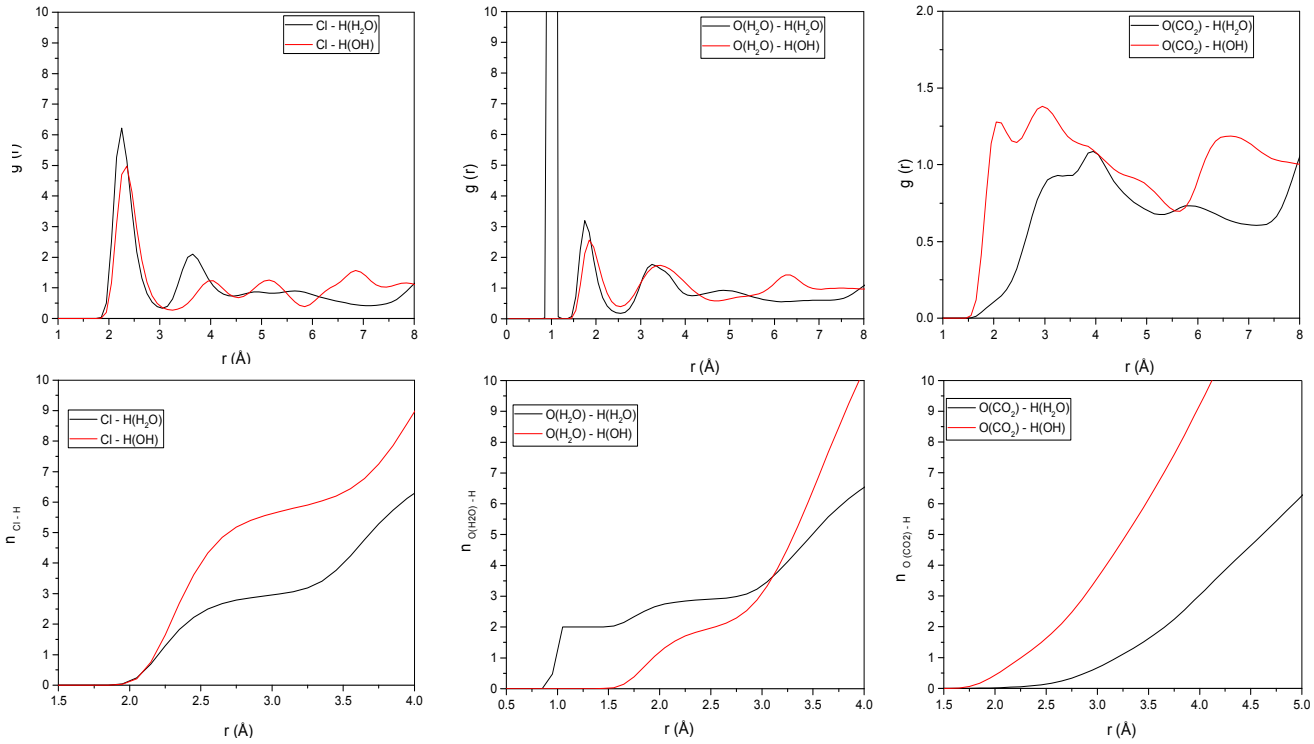
An average number of hydrogen bonds per interlayer water molecule = 3.6

Figure S 43- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 216 CO_2 and 432 H_2O in the interlayer region.



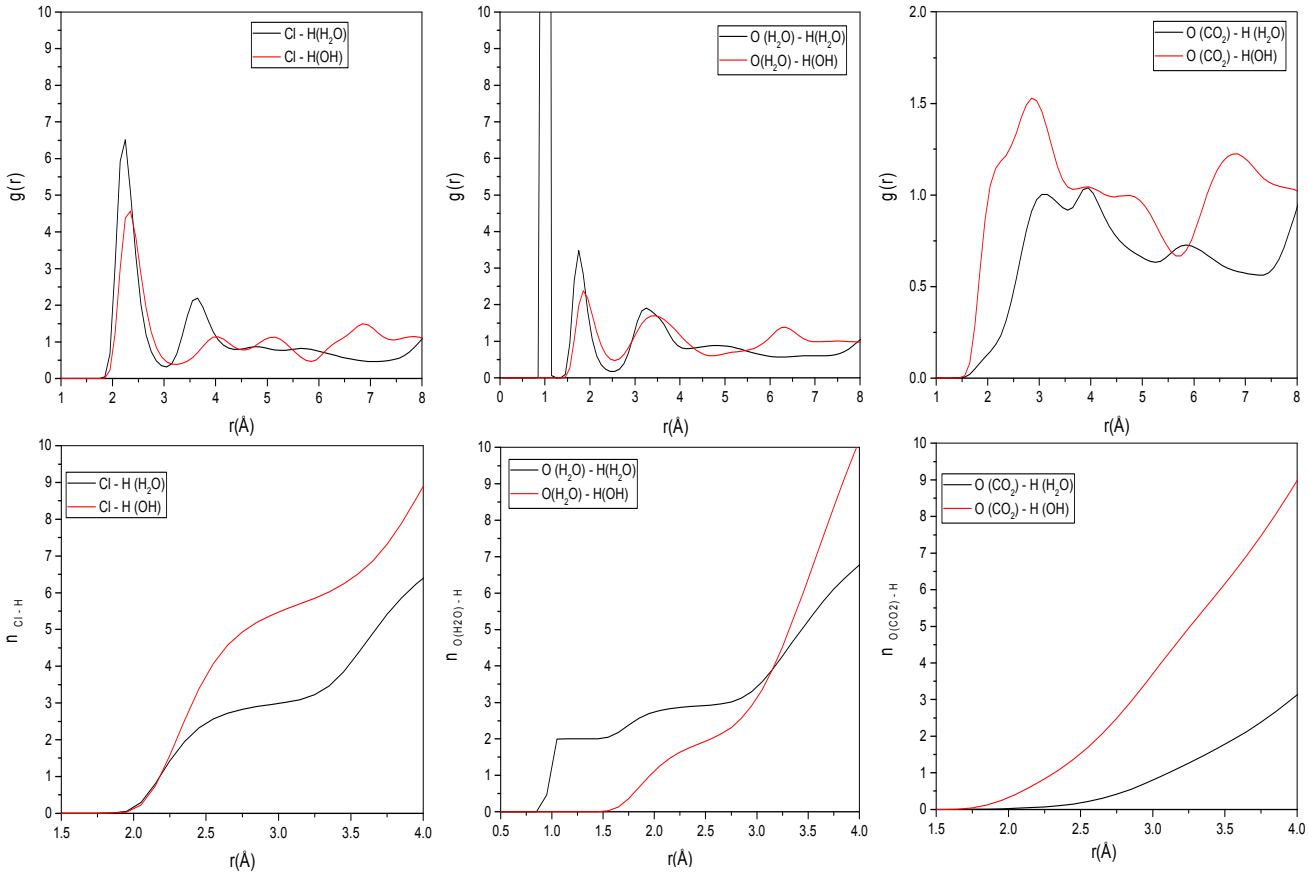
An average number of hydrogen bonds per interlayer water molecule = 3.8

Figure S 44- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 432 CO_2 and 432 H_2O in the interlayer region.



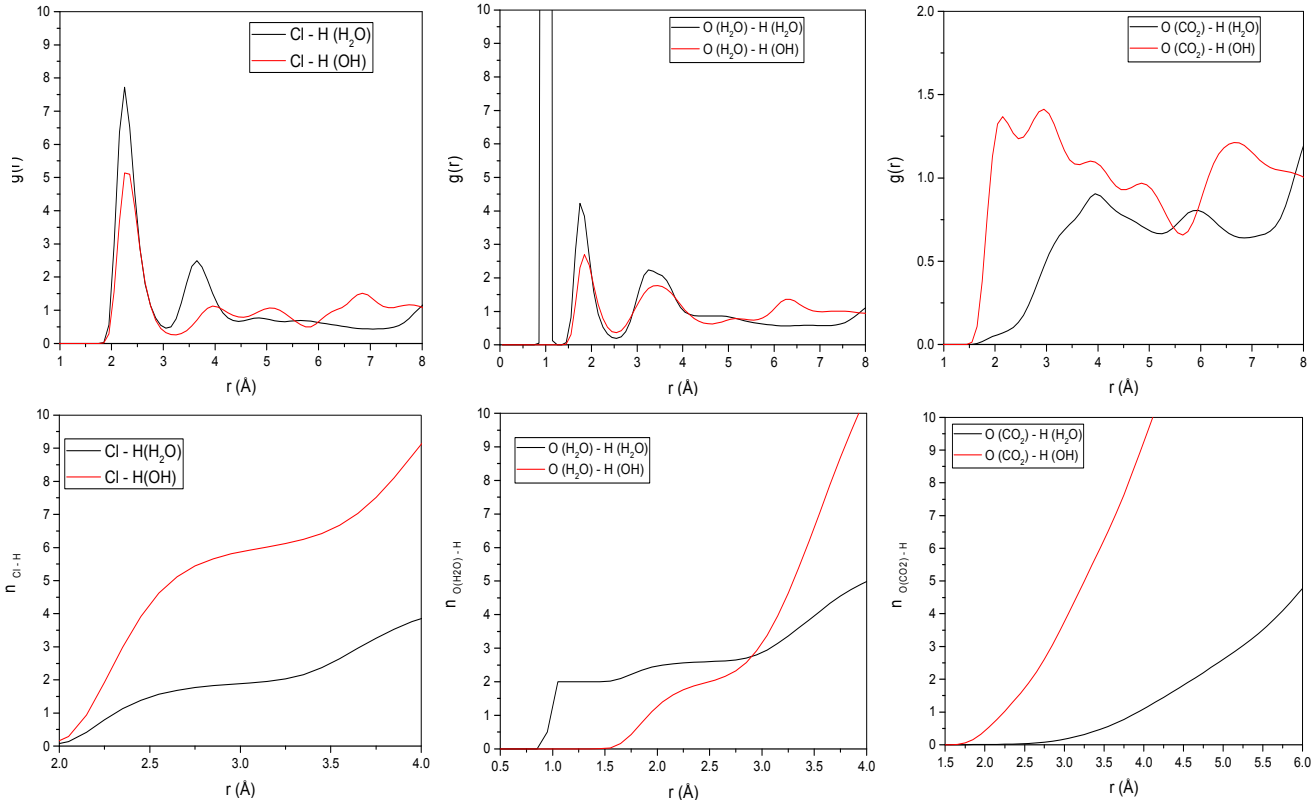
An average number of hydrogen bonds per interlayer water molecule = 3.7

Figure S 45- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 36 CO_2 and 864 H_2O in the interlayer region.



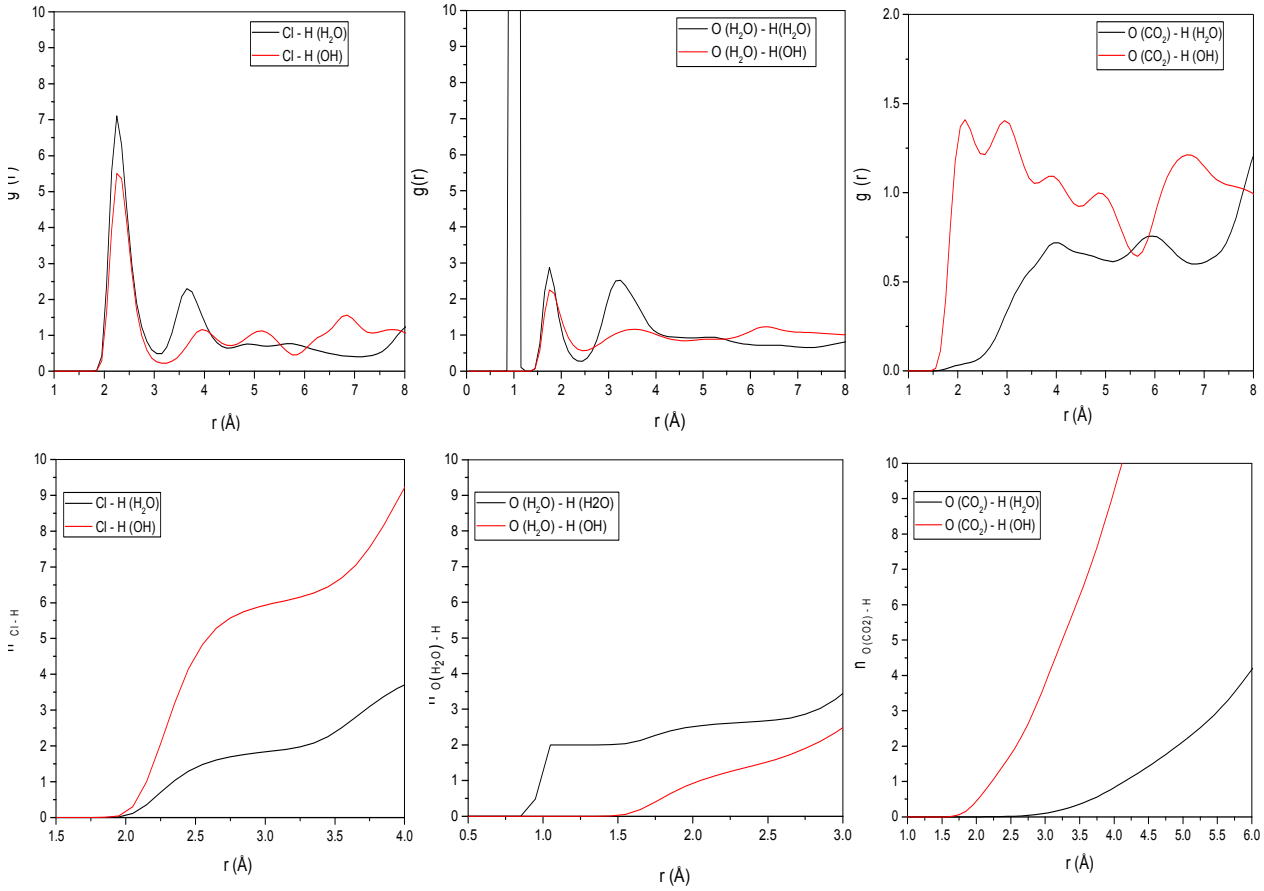
An average number of hydrogen bonds per interlayer water molecule = 3.9

Figure S 46- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 84 CO_2 and 864 H_2O in the interlayer region.



An average number of hydrogen bonds per interlayer water molecule = 3.6

Figure S 47- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 216 CO_2 and 864 H_2O in the interlayer region.



An average number of hydrogen bonds per interlayer water molecule = 3.5

Figure S 48- Radial distribution functions and integrated nearest-neighbor coordination numbers for Cl^- - H pairs and O (H_2O) - H pairs and O (CO_2) – H pairs in the interlayer of Mg/Al Cl^-- hydrotalcite computed from MD simulations. There are 432 CO_2 and 864 H_2O in the interlayer region.