

Electronic Supplementary Information (ESI) for

First-principles molecular dynamic simulation of the $\text{Ca}_2\text{UO}_2(\text{CO}_3)_3$ complex in water

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Figure S1. The orbital-resolved local density of states on the U atom from a snapshot of the $\text{Ca}_2\text{UO}_2(\text{CO}_3)_3$ complex in water. (Energy is relative to the Fermi level).

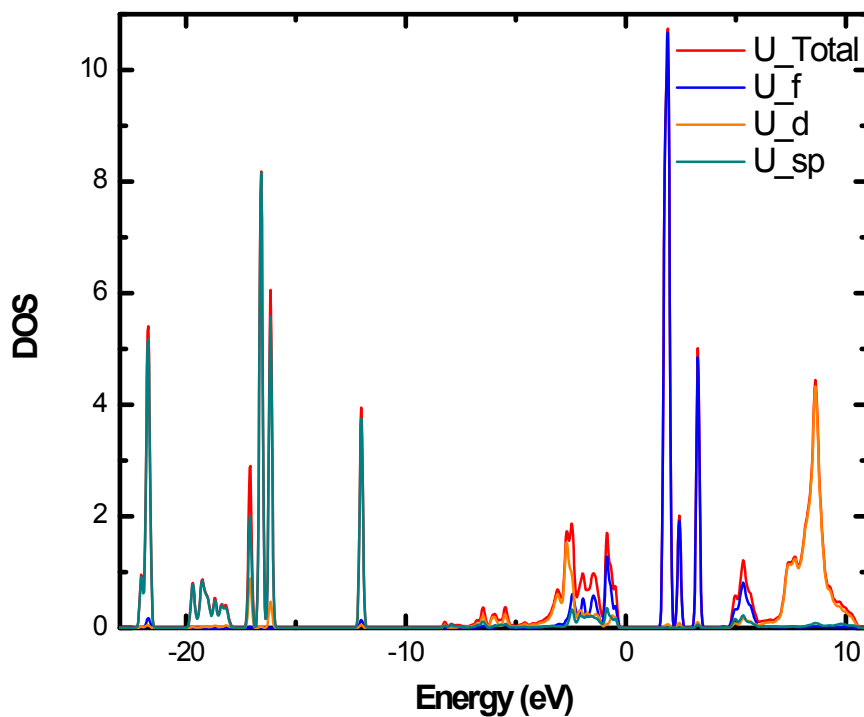
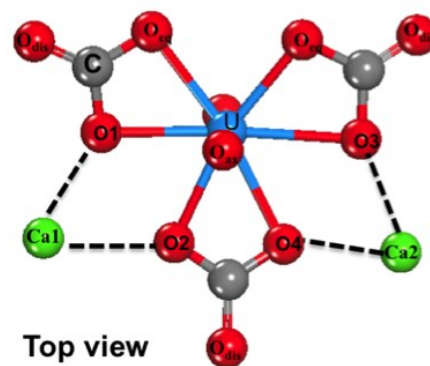
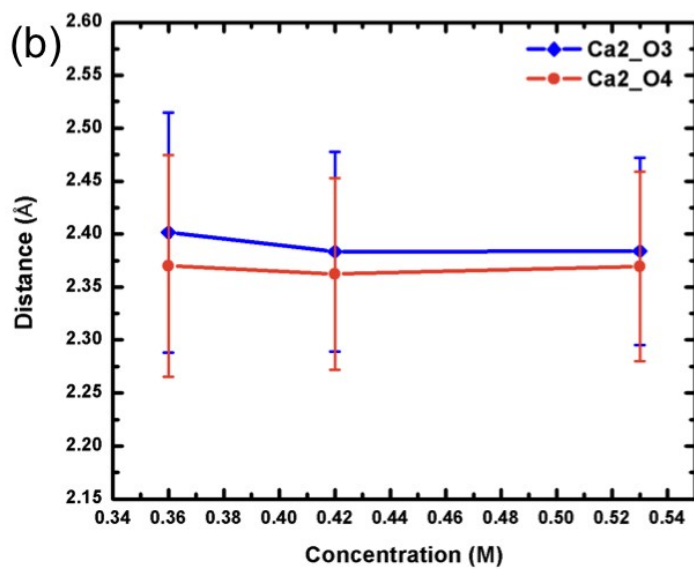
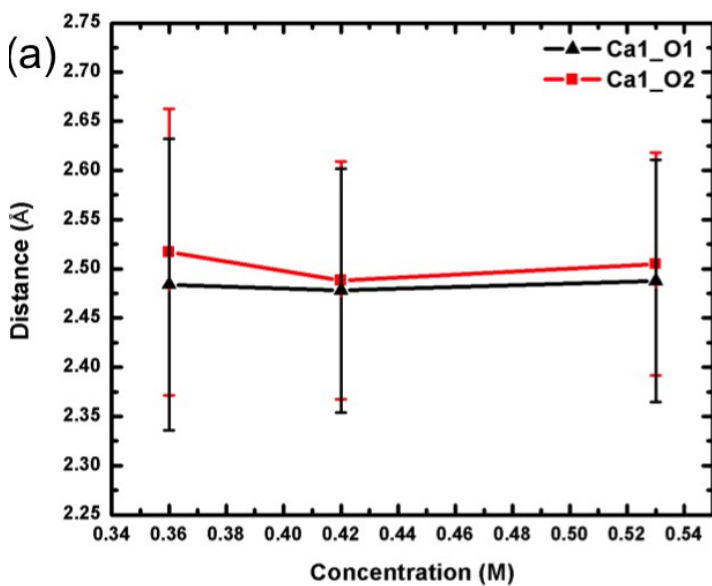


Figure S2. Averages and standard deviations of the four Ca-O_{eq} distances of the Ca₂UO₂(CO₃)₃ complex in water at three different concentrations over 15ps trajectories.



A snapshot of the $\text{Ca}_2\text{UO}_2(\text{CO}_3)_3$ complex in water: in VASP POSCAR format that can be visualized by many free programs such as Molden.

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0.889902055264	0.418224364519	0.595628499985
0.775594592094	0.121288031340	0.438056081533
0.388847053051	0.788352370262	0.074697978795
0.427755832672	0.880098044872	0.032998539507
0.655659794807	0.975299358368	0.751982092857
0.582507014275	0.003643929958	0.830064952374
0.710387885571	0.115723028779	0.634252607822
0.657184958458	0.208803296089	0.651875674725
0.852961421013	0.870045125484	0.473509758711
0.929200470448	0.895072221756	0.400887757540
0.040332179517	0.676624059677	0.455325692892
0.126489236951	0.636001348495	0.412106931210

0.789947688580	0.817655086517	0.620528936386
0.882632553577	0.878605127335	0.616486489773
0.381726771593	0.478561133146	0.360617876053
0.732322394848	0.555097639561	0.393235623837
0.538720726967	0.516548931599	0.658537805080
0.551728963852	0.509299874306	0.461286693811
0.306106209755	0.455522686243	0.585586428642
0.763999223709	0.566294193268	0.639546990395