Probing the structure and stability of calcium carbonate prenucleation clusters

Aaron R. Finney and P. Mark Rodger, *Faraday Discuss.*, DOI: 10.1039/c2fd20054f

Supplementary Information

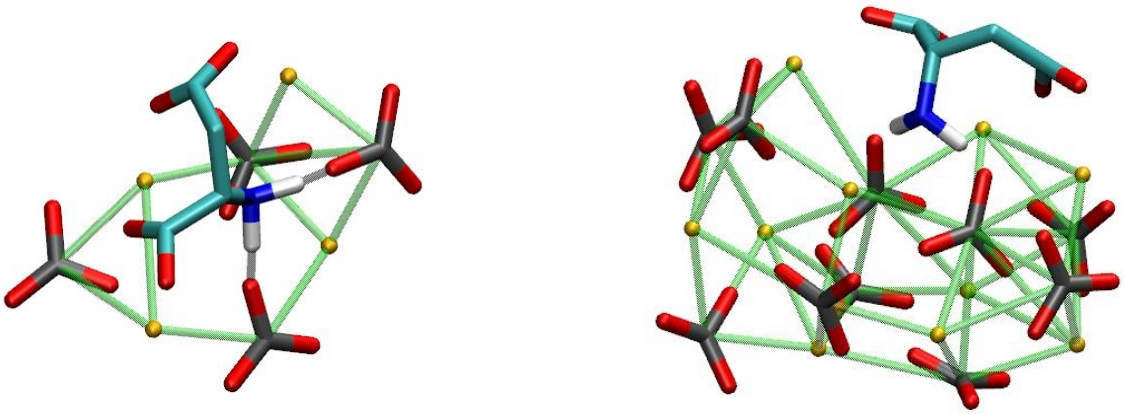


Figure S1 Minimum energy clusters found from random structure generation and subsequent optimisation of ten thousand structures from the gas phase. Left shows a $4(CaCO_3 \cdot H_2O) \cdot ASP$ cluster, while the structure on the right is for $10(CaCO_3 \cdot H_2O) \cdot ASP$. Atoms are coloured: red for oxygen, black (carbonate) and cyan (ASP) for carbon, yellow for calcium, blue for nitrogen and white for hydrogen. ASP backbone hydrogens and optimised water have been excluded for clarity.

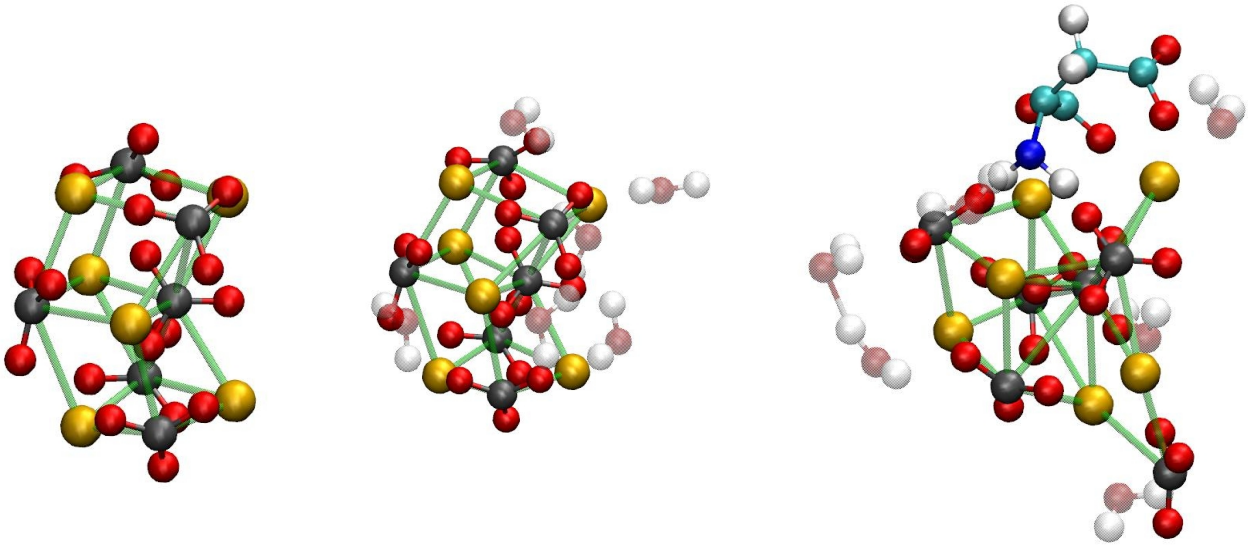
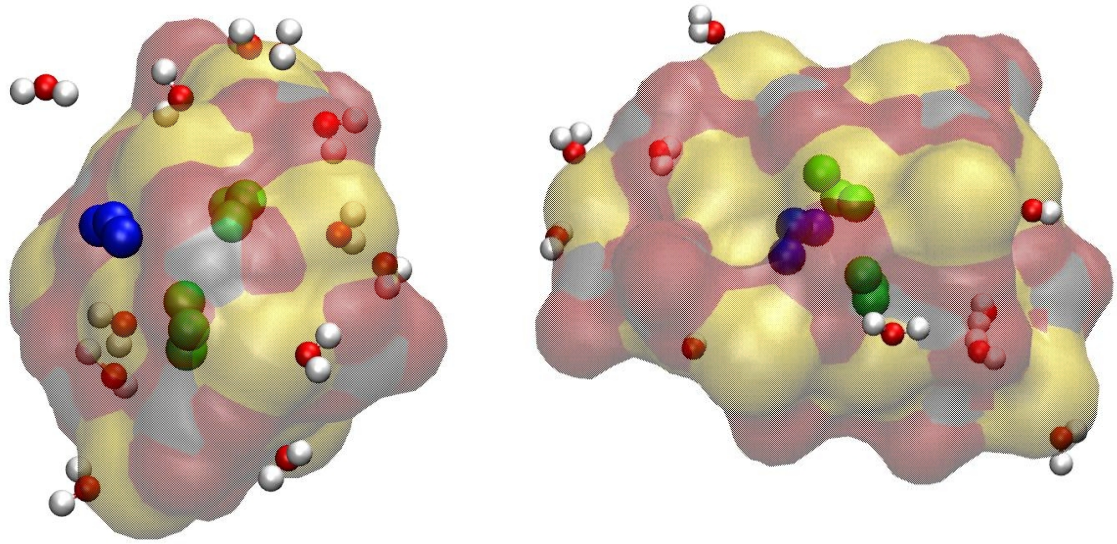


Figure S2 Minimum energy clusters found from random structure generation and subsequent optimisation. Left shows a cluster containing $6CaCO_3$, centre shows $6CaCO_3 \cdot H_2O$ while the structure on the right is for $6(CaCO_3 \cdot H_2O) \cdot ASP$. Atoms are coloured as for those in figure S1, and water is shown for completeness.



a *b*

Figure S3 Initial (a) and final (b) structures of a $15CaCO_3{\cdot}H_2O$ cluster from a 5 ns simulation in water. Carbon, oxygen, calcium and hydrogen are coloured black, red, yellow and white respectively. Highlighted are two water molecules (green) which reside below the cluster surface throughout the simulation, and one water molecule (blue) which initially resides at the surface of the cluster, but is absorbed below the surface at ~80 ps.

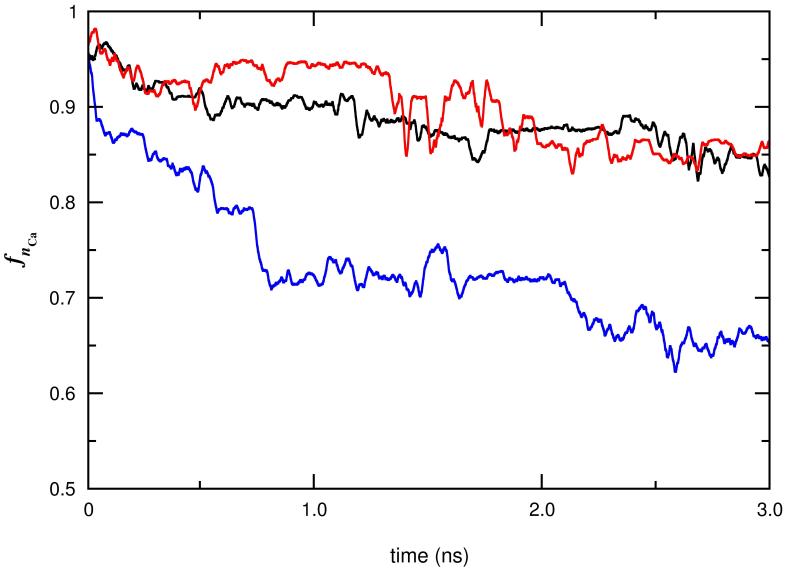


Figure S4

Fraction of maximum coordination number, $f_{\mathbf{n}_{Ca}}$, for minimum energy (*in vacuo*) clusters containing 15 $CaCO_3$ units, simulated in water. Anhydrous (red), hydrous (black) and ASP inclusive (blue) clusters have been simulated.