UNIVERSITY OF TWENTE.

wetsus
european centre of excellence for sustainable water technology

Molecular Dynamics simulation of calcium carbonate nucleation process under the effect of magnetic field

Background

Calcium carbonate can be created in several mineral forms by the reaction of dissolved carbon dioxide in water with calcium ions through biomineralization process. The details of the prenucleation form of calcium carbonate are still under investigation. Based on the latest MD simulation studies, these stable prenucleation clusters of calcium carbonate (aka "DOLLOPs" - dynamically ordered liquid like oxyanion polymers)are constantly evolving, yet stable ionic polymers consisting of linear or branched chains of cations and anions held together by only ionic interactions (see Fig. 1). Also, after the nucleation of calcium carbonate, formation of amorphous calcium carbonate (ACC) and its subsequent transformation into crystalline phases is in progress.

There is still much to be learned about the formation and development of DOLLOPs into ACC and the different polymorphs of calcium carbonate. An MD study can lead to important information on their chemistry like growth rates and equilibrium constants. The goal of this project is to extract this kind of practically relevant information from MD simulations starting from several different, stable DOLLOP configurations so that this data can then be compared to experimentally derived chemical and physical parameters.

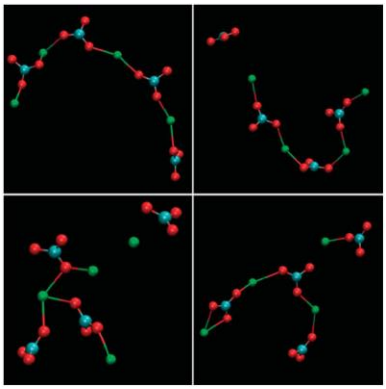

Figure 1: Structures of the four formula unit prenucleation clusters[1].

Requirements

The ideal candidate has had previous experience and working knowledge with Molecular Dynamics simulation software LAMMPS, especially simulation of water models (particularly SPC/Fw water model). Taking initiative and good communication are important. A good lap-top or desktop computer with fast internet access to serve as terminal for the simulation server is required.

Starting date: ASAP

Duration: At least 3 months; can eventually be extended to a master thesis (6 months)

Research institute

This project is a cooperation of University of Twente and Wetsus, Centre of Excellence for Sustainable Water Technology, located in Leeuwarden. This project is part of the Wetsus Applied Water Physics theme. The institute employs people from vastly different fields and backgrounds and combines this knowledge for the best results, with an international environment where the working language is English, so fluency in this language is required. Due to the corona pandemic, we will attempt to allow the candidate to work from home via remote login as much as possible. The researcher will be supervised by Talie Zarei (Wetsus) and Profs. Wouter den Otter and Herman l. Offerhaus (University of Twente).

Application

If you are interested in this project, please contact Talie Zarei at Wetsus (talie.zarei@wetsus.nl) or Prof. Dr. Herman l. Offerhaus at University of Twente (h.l.offerhaus@utwente.nl). for more information or directly apply by sending your CV to the same address. If In absence of an Erasmus grant the internship/MSc thesis includes a reimbursement of €175.- per month for living expenses.

[1]. Demichelis, R., et al., *Stable prenucleation mineral clusters are liquid-like ionic polymers.* Nature communications, 2011. **2**(1): p. 1-8.