PAWSEY supercomputing centre

PARTNER INSTITUTION

Curtin University

USING QUANTUM MECHANICS TO UNLOCK THE SECRETS OF CORAL

Coral reef with yellow coral turbinaria mesenterina at the bottom of tropical sea, underwater

PROJECT LEADER
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SYSTEM
MAGNUS

TIME ALLOCATED
27,000,000 HOURS

AREA OF SCIENCE
CHEMISTRY

APPLICATIONS USED
LAMMPS
CP2K
Plumed
GULP
Tinker
OpenMM

Biomineralisation is one of the most important processes for mineral formation in the natural world – taking place in everything from coral reefs to bones and teeth in the human body. One of the most widespread of these minerals is calcium carbonate. Despite being so prevalent, relatively little is known about the formation of these minerals. Professor Julian Gale from Curtin University is leading a team of researchers to uncover the secrets of these common but little-understood processes.

Professor Gale's project focuses on the family of biominerals that are pivotal to processes such as long term carbon sequestration, as well as those responsible for the minerals that occur in the human body. Their objective is to understand how such minerals assemble at the atomic level – something that is hard to achieve in the laboratory, but is becoming possible using computer models.

2018

ATOMISTIC SIMULATION OF MINERALS, MATERIALS AND GEOCHEMISTRY

THE CHALLENGE

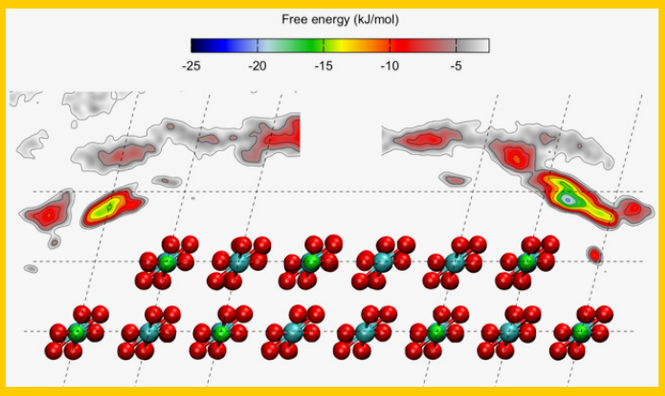
Crystals are the basis of much of the solid matter around us. Understanding how they form from their component molecules and/or ions in solution has long been a challenge. If we were able to control this process then we would be able to limit the formation of scale that blocks pipes and vessels that costs industry in lost productivity, as well as being able to design new materials such as pharmaceuticals. In the context of minerals specifically, the formation of crystals is one of the processes by which systems are purified in industry and in nature this goes to form everything from sand on the beach, to teeth.

"One of the most widespread minerals in the environment is calcium carbonate, and its formation is especially important since it can be found everywhere from the limestone cliffs of the Nullarbor to scale in kettles & industrial pipelines. Closely related minerals are also being considered as candidates for long-term geosequestration," says Professor Gale.

Despite being so common, it is very difficult to directly study the formation process of biominerals like calcium carbonate due to the extremely small size of the species involved and their low concentration. Recently, supercomputing has helped researchers produce computer models to simulate the early stages of formation.

"With the advent of petascale computing, it has now become feasible to directly test some of the results of empirical force models against what should be, in principle, more reliable methods based on quantum mechanics, in which the interactions come from the fundamental laws of physics," says Professor Gale.

However, these simulations can be extremely computationally intensive. Professor Gale says that



Free energy iso-surfaces for carbonate adsorbing at the obtuse (left) and acute (right) calcite steps. The calcite structure is shown with calcium, carbon and oxygen in green, blue and red, respectively. Reference for the Figure is M. De La Pierre et al, Angewandte Chemie, 56, 8464 (2017).

while most simulations of this kind to date have involved tens of thousands of calculations, his team's project aims to model many millions of steps instead.

"The challenge is not to be able to run a single calculation, but that the parallel scaling needs to be sufficient that each calculation would only take a few seconds to execute in order to make long runs feasible."

THE SOLUTION

Using Magnus, Professor Gale and his team can perform the rapid parallel calculations needed to simulate millions of steps in a practical timeframe. "Choice of algorithm and some of the unique features of the code that we use, CP2K, are the key to being able to exploit the computing power of the Pawsey Centre and to achieve the objectives of our project," says Professor Gale.

"During the course of the project, we have managed to tune the computational settings to gain in excess of an order of magnitude in productivity (i.e. time per step) without adversely affecting the quality of the results."

Combining supercomputing processing power with advanced codes and algorithms, Professor Gale and his team are able to model the binding of calcium and carbonate atoms at more realistic conditions.

OUTCOME

"Our simulation is one of the most extensive quantum mechanical molecular dynamics studies ever performed in the world to date," says Professor Gale. The simulation highlights some significant differences between the quantum mechanical and empirical simulations that will now be explored.

"The results from this project will lead to improved force field models that better capture some of the important features of the quantum mechanics."

As a result of this project, one of the most common but least understood building blocks of the world is now being uncovered.