# Towards a holistic understanding of carbonate (bio)mineralisation controls

| | |
|---|---|
| **Primary supervisor:** | *Prof. Julie Cosmidis, department of Earth Sciences*<br>https://www.earth.ox.ac.uk/people/julie-cosmidis<br>https://www.cosmidislab.com/ |
| **Co supervisor(s):** | *Prof. Ros Rickaby, department of Earth Sciences*<br>*https://www.earth.ox.ac.uk/people/ros-rickaby*<br>*Prof. Sarah Waters, Mathematical Institute*<br>*https://people.maths.ox.ac.uk/waters/Waters/Dr_Sarah_Waters.html*<br>*Dr. Luca Stigliano, department of Earth Sciences*<br>*https://www.earth.ox.ac.uk/people/luca-stigliano* |
| **Key words:** | Carbonates, biominerals, carbon capture and storage, Raman spectroscopy, modelling, Machine Learning |
| **Research theme(s):** | • Earth Resources<br>• Oceanography, Climate and Palaeoenvironment |
| **Eligible courses for this project:** | • Environmental Research (NERC DTP)<br>• Intelligent Earth (UKRI CDT)<br>• Interdisciplinary Bioscience (BBSRC DTP) |

## Overview

Calcium-carbonates ($CaCO_3$) are climate-controlling minerals, acting as long-term sinks in the biogeochemical carbon cycle, and playing the role of stable carbon stores in many carbon capture, utilisation and storage (CCUS) technologies. $CaCO_3$ minerals formed either through low-temperature chemical precipitation or as biominerals by calcifying microorganisms are also increasingly used in applications such as carbon-negative concrete, cements, and other materials, potentially enhancing the economic profitability of CCUS. The design of effective CCUS and material applications requires the ability to predict and control both the rate at which $CaCO_3$ (bio)minerals form, and the mineralogical properties (e.g., crystal structure, morphology or size) of the particles formed, as these factors can significantly impact the efficiency of carbonate mineralization and the long-term stability of its products. However, we still lack a comprehensive understanding of how multiple environmental variables control $CaCO_3$ mineralization. Indeed, carbonate crystallisation is under the influence of many physicochemical variables such as temperature, pH, supersaturation and salinity, as well as of a great number of inorganic and organic species (called additives) that can act as inhibitors or promoters of nucleation and growth (Figure 1). While the impacts of these factors on $CaCO_3$ mineralization have been studied individually, their combined effects remain poorly known. In fact, our current understanding is largely based on empirical studies that investigate the effects of these factors in isolation, providing findings that cannot be easily extrapolated to different conditions, and failing to capture the complexity of natural and engineered systems where multiple variables interact.

This DPhil project will address this knowledge gap by deploying new high-throughput experimentation and *in-situ* mineralogical characterization methodologies (High-Throughput Screening Raman), that will allow us to rapidly perform thousands of $CaCO_3$ (bio)mineralization experiments, covering a wide multi-dimensional space of physicochemical variables as well as thousands of inorganic and molecular additives. The large datasets thus assembled will be used to build mathematical models and Machine Learning algorithms that will aim at gaining a mechanistic and predictive understanding of how multiple physicochemical parameters and organic molecules control the mineralogical properties and growth rates of carbonate minerals in complex chemical systems as well as in calcifying organisms.

Potential outcomes: The project results may eventually contribute in the development of more effective CCUS strategies, upporting efforts towards sustainable carbon management solutions. By improving our understanding of the role of inorganic and molecular additives in controlling the mineralogical properties of carbonate crystals, this project may furthermore enable the development of new engineering approaches for the design of improved $CaCO_3$ particles for construction and other material applications.

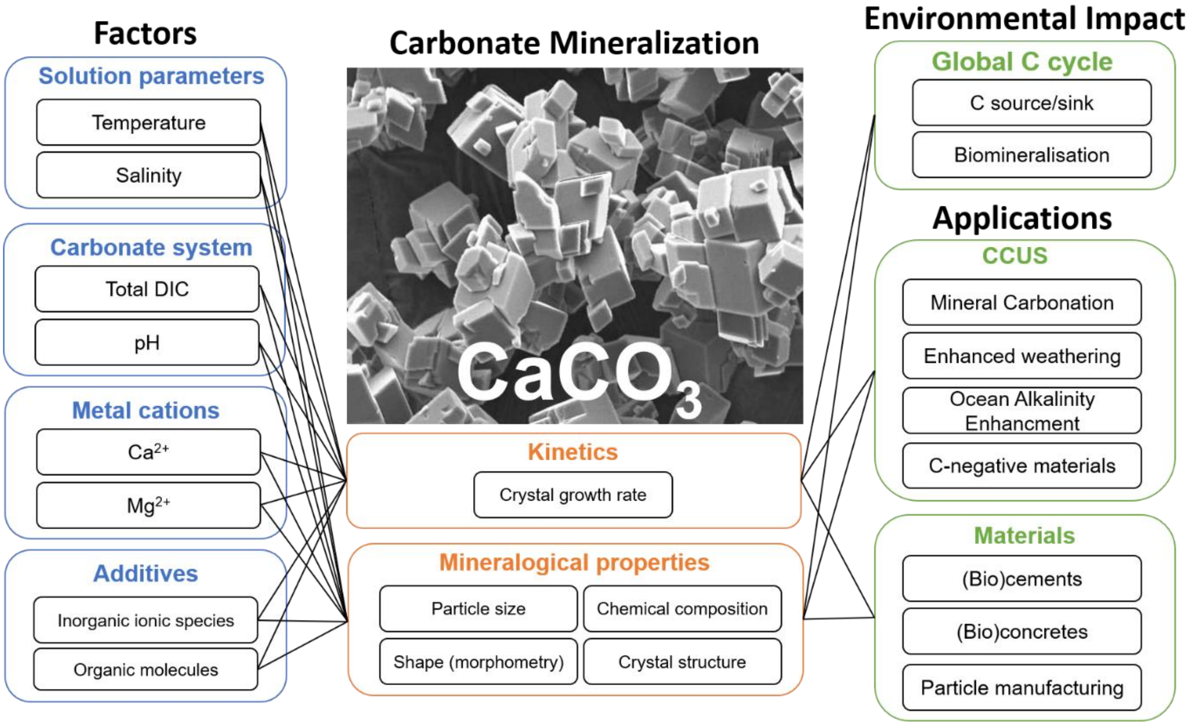


*Figure 1:* Multiple factors influence $CaCO_3$ mineralization kinetics and properties, affecting their efficiency in CCUS and material applications.

## Methodology

Experimental: Preparation of carbonate mineralization experiments in abiotic conditions as well as in cultures of eukaryotic and microbial calcifiers. High-throughput precipitation experiments in multi-well plates. Extraction of biomineral-controlling polysaccharides from calcifiers.

Mineralogical characterization techniques: High-throughput Screening Raman spectromicroscopy, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Measurements of particle growth kinetics in microfluidic flow cell systems.

Modelling: Mathematical modelling, model reduction, analytical and numerical solution of differential equations

Machine Learning: supervised ML algorithms (e.g., Random Forests, Support Vector Machines, Gradient Boosting Machines, Artificial Neural Networks including Graph Neural Networks)

Please note that not all expertise in the different areas are required, as the project can be tailored to match the expertise and research interests of the applicant.

## Timeline

**Year 1**: Doctoral training courses, literature review, laboratory and analytical training, first experiments.
**Years 2 and 3**: Laboratory experiments, analytical work, presentation of research at national conferences.
**Year 4**: Data integration, thesis completion, writing of papers for international journals, presentation of research at an international conference.

## Training & Skills

The student will be trained in laboratory techniques specific to the project (carbonate mineralization experiments, culturing), as well as in a range of analytical techniques for mineralogical and material characterization (e.g., Raman spectroscopy, electron microscopy). Depending on previous experience and skills, training will be also provided on the computational aspects of the project (mathematical modelling, machine learning). The DPhil programme will also provide opportunities for soft-skills training, such as planning and managing a research project, interpreting data and presenting scientific results, and writing scientific papers for publication.

## References & Further Reading


Cosmidis, J., 2023. Will tomorrow's mineral materials be grown? Microbial Biotechnology 16, 1713–1722. https://doi.org/10.1111/1751-7915.14298

Lee, R.B.Y., Mavridou, D.A.I., Papadakos, G., McClelland, H.L.O., Rickaby, R.E.M., 2016. The uronic acid content of coccolith-associated polysaccharides provides insight into coccolithogenesis and past climate. Nat Commun 7, 13144. https://doi.org/10.1038/ncomms13144

Lin, J.-Y., Garcia, E.A., Ballesteros, F.C., Garcia-Segura, S., Lu, M.-C., 2022. A review on chemical precipitation in carbon capture, utilization and storage. Sustainable Environment Research 32, 45. https://doi.org/10.1186/s42834-022-00155-6

Niu, Y.-Q., Liu, J.-H., Aymonier, C., Fermani, S., Kralj, D., Falini, G., Zhou, C.-H., 2022. Calcium carbonate: controlled synthesis, surface functionalization, and nanostructured materials. Chemical Society Reviews 51, 7883–7943. https://doi.org/10.1039/D1CS00519G

## Further Information

Contact: Prof. Julie Cosmidis (Julie.cosmidis@earth.ox.ac.uk)