EARTHSCIENCES

Protein specific mineralisation and exceptional fossils

Primary supervisor:	Ross Anderson
Co supervisor(s):	Julie Cosmidis Jani Bolla (Biology) Piyush Sriwastava (Museum of Natural History)
Key words:	Biomineralisation, AI, proteomics
Research theme(s):	• Oceanography, Climate, Palaeoenvironment • Palaeobiology and Evolution
Eligible courses for this project:	• DPhil in Earth Sciences • Environmental Research (NERC DTP) • Intelligent Earth UKRI CDT

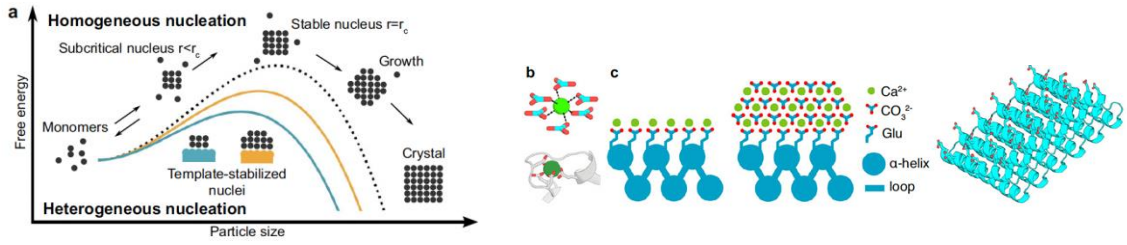
Overview

Exceptionally preserved fossil assemblages that preserve not only the biomineralised tissues of organisms but also their soft parts, including internal organs, are critical for interpreting the history of life on our planet. Minerals have been argued to be important in exceptional preservation via their replication of soft tissues (e.g., pyritization, phosphatisation) and via their conservation of organic molecules (e.g., enhanced polymerization via clay-organic bonds). However, the molecular-scale processes underpinning these organic-mineral interactions remain poorly understood. Recent advances in protein structure prediction using machine learning algorithms have hinted how mineralisation may be controlled by protein surface structure. This project aims to establish how protein structure influences protein-mineral interactions important to exceptional preservation of fossils.

This DPhil will:

(1) Determine the protein templates that promote the heterogeneous nucleation of minerals.

(2) Synthesise experimentally minerals in the presence of designed proteins, uncovering the underpinning mechanisms of mineralisation in exceptional fossil preservation.



(Davila Hernandez et al. 2023)

Methodology

Modelling a protein surface with bond parameters similar to the dominant face of mineral(s) from exceptional fossil assemblages e.g., clays, sulphides, phosphates. Using an AI based platform (Rosetta Macromolecular Modelling Suite), design the protein templates with the required surface properties. Obtain the gene fragments encoding the designed peptide sequences, express them in bacteria (E. coli etc), and purify the required protein.

Use extracted protein and interact it with pore fluid chemistry appropriate to the host rock of exceptional fossilisation. Characterize the minerals nucleated on the protein surface.

Timeline

Years 1: DTP Training modules, mini research project providing training on computational approaches to protein design and deep learning AI methods to extract the sequence motifs from natural proteins that are involved in mineralisation.

Year 2: Design the protein templates with required surface properties, decode amino acid sequence and obtain synthetic gene fragments for overexpressing these designed templates for further characterisation. Wet lab training and optimising the expression and purification of proteins. Biophysical analyses of purified proteins, these include CD spectroscopy, mass spectrometry, and X-ray crystallography.

Year 3: Perform nucleation experiments with the purified proteins and pore fluid representative for host rock. Perform TEM to determine the particle morphology and size. Determine the mechanism of mineralisation.

Year 4: Data analysis, writing papers, thesis, and attending conferences.

Training & Skills

Training and skills in geochemical data collection, database management, quantitative analysis of databases, writing, and forming logical arguments.

References & Further Reading

Anderson, R.P., Tosca, N.J., Gaines, R.R., Mongiardino Koch, N., Briggs, D.E.G., 2018. A mineralogical signature for Burgess Shale-type fossilization. *Geology* 46 (4), 347–350.

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Further Information

Contact: Ross Anderson (ross.anderson@oum.ox.ac.uk)