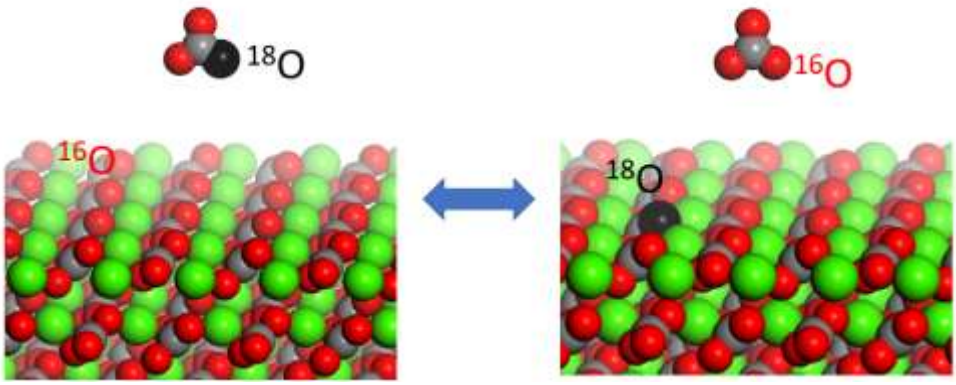
Stable isotope fractionation in minerals as a tool for climate reconstruction: insights from molecular modelling.

Lead Supervisor: Ricardo Grau-Crespo, University of Reading, Department of Chemistry.
Email: r.grau-crespo@reading.ac.uk

Co-supervisors: Zuowei Wang, Department of Mathematics and Statistics, University of Reading; Marco Sacchi, Department of Chemistry, University of Surrey; Dominik Fleitmann, Department of Environmental Science, University of Basel.

We are looking for a talented and motivated PhD student to work on a multidisciplinary project about modelling stable-isotopic exchange between minerals and aqueous solutions. Subtle changes in the concentration of stable isotopes in natural archives such as sediments in oceans or polar ice caps can be precisely measured to reconstruct climate history. For example, by comparing the ratio of oxygen isotopes in shells found in marine sediments, it is possible to determine the seawater temperature over time, because the isotope ratio is affected by temperature. The interpretation of isotope records requires a detailed understanding of the complex processes governing isotope exchange, which has motivated the development of theoretical models to predict and rationalise the fractionation of stable isotopes between different phases. Such approaches are typically based on molecular-level considerations: the vibrational behaviour of atoms depends on the isotopic masses involved, affecting equilibrium free energies and kinetic barriers. Molecular modelling techniques based on quantum chemistry or classical forcefields, can then be used to predict the fractionation of stable isotopes between phases. Significant progress has been achieved in recent years in this research direction, but some important challenges remain, because drastic approximations must often be made to avoid the huge computational cost of atomistic-level simulations. In this project, we will take advantage of recent major advances in molecular modelling, based on the incorporation of machine-learning algorithms, to overcome these limitations and achieve a faster and more accurate prediction of stable isotope fractionation. Drawing on the team's experience modelling carbonate minerals with geochemistry applications in mind [1-3] and in applying machine-learning algoritms to accelerate quantum-chemistry modelling [4-6], we will develop new methods for isotope fractionation prediction with the potential to transform the interpretation of stable-isotope records.



The ratio of oxygen isotopes in shells made of calcium carbonate can be used to reconstruct past temperatures of seawater.

Training opportunities:

There will be distinctive training opportunities for the student in molecular modelling and machine learning via our group's association with the UK's HPC Materials Chemistry Consortium to access the ARCHER2 national supercomputer facility. The UoR is one of nine UK university leaders in the field of molecular modelling who run the MMM Hub (https://mmmhub.ac.uk) and the Young supercomputing facility, which also provides access to excellent training and support opportunities. The student will also take advantage of the cohort-based nature of the Scenario partnership and the opportunities for training in more general themes of environmental science.

Student profile:

We are looking for a student with a master-level degree, preferably in Chemistry or Physics or related subject (other backgrounds, like Maths, Computer Science, or Earth Sciences, could be considered, depending on the student's track record). Previous experience in one or more of the following areas would be considered an advantage: a) molecular modelling, b) machine learning c) geochemistry or mineralogy.

References: (optional)

1. SD Midgley, JO Taylor, DO Fleitmann, R Grau-Crespo. *Chemical Geology* 553 **(2020)** 119796.
2. SD Midgley, D Di Tommaso, D Fleitmann, R. Grau-Crespo. *ACS Earth and Space Chemistry* 5 **(2021)** 2066−2073.
3. SD Midgley, D Fleitmann, R Grau-Crespo. *Geochimica et Cosmochimica Acta* 324 **(2022)** 17-25.
4. LM Antunes, R Grau-Crespo, KT Butler. *npj Computational Materials* 8 **(2022)** 44.
5. SD Midgley, S Hamad, KT Butler, R Grau-Crespo. *Journal of Physical Chemistry Letters* 12 **(2021)** 5163-5168.
6. JJ Plata, V Posligua, A Marquez, JF Sanz, R Grau-Crespo. *Chemistry of Materials* 34 **(2022)** 2833–2841.

https://research.reading.ac.uk/scenario/