GÉOSCIENCES ENVIRONNEMENT TOULOUSE

La Terre est notre laboratoire

Post-doc position in Path Integral Molecular Dynamics applied to Geochemistry

Position duration : 1 year renewable, starting date : March 2020.
Coordinator: Merlin Méheut, associate professor (merlin.meheut@get.omp.eu) +33 5 61 33 26 17
Partners : Magali Benoît (CEMES), Rodolphe Vuilleumier (ENS Paris), Mark Tuckerman (NYU)
Location of the position : Géosciences Environnement Toulouse (GET), « Stable Isotopes Geochemistry » group, Observatoire Midi-Pyrénées, Université Paul Sabatier (Toulouse, France)

Scientific context

Isotopic compositions of natural phases constitute a tool of primary importance to assess geological history. Recent progresses in mass spectrometry and analytical chemistry have enabled the detection of isotopic variations of a host of elements (e.g. Fe, Mg, Ca, Li, Zn), opening the path to numerous applications. In particular, Ca isotopes have shown their potential for medical applications (early diagnosis of decalcification), to assess mechanisms occuring at the soil-plant interface, or to assess the Ca cycle in the environment.

To take the full extent of these new measurements, it is necessary to precisely constrain the isotopic effect associated with elementary processes occuring at the atomic level. In this perspective, the fractionation of isotopes reached at thermodynamical equilibrium (called equilibrium fractionation) between two phases (between one mineral and a dissolved species, or between two dissolved species) is of particular interest.

It is possible to estimate isotopic fractionation based on atomistic modeling by estimating the thermo-kinetic properties of atoms in a given bonding environment. For solids, these properties are generally estimated based on the harmonic approximation, starting from the vibrational frequencies of the mineral (e.g. Méheut and Schauble 2014). For liquids, we have developed an approach based on path integral molecular dynamics (PIMD, Dupuis et al 2017). This approach, which was applied to Li isotopes, is computationally very expensive, and that is why it has been limited so far to the use of empirical potentials to describe atomic interactions.

Our primary goal is to set an affordable numerical scheme to compute equilibrium fractionation properties of any material, in particular dissolved species, based on path integral molecular dynamics methods, but with atomic bonding described by ab initio electronic structure computations (instead of empirical potentials), so as to render its application to virtually any case. This approach will be first tested on the Ca^{2+}-H_2O system for which experimental data exist.

Description of the position:

The work of the researcher will be first to set up path integral molecular dynamics on a Ca^{2+}-H_2O system, with empirical potentials (with the CP2K code), in order to compute Ca isotopes fractionation properties for this system. Then, with the aim to reduce the computing time, we will consider two schemes:

- setting up path integral Langevin dynamics on the same system.
- setting up the « ring polymer contraction » approach.

The postdoctoral researcher will be responsible for the first approach, and for the development of fractionation properties calculations based on this approach. At last, the researcher will set up the Langevin dynamics calculations (or the ring polymer contraction, depending on which will be shown more promising) based on an ab initio description of atomic interactions, with the CP2K code.

For further information about the project, please contact:
Merlin Méheut : merlin.meheut@get.omp.eu

To apply for this position, please connect to the following link : http://bit.ly/37iNLGc
CV and motivation letter will be requested.

Géosciences Environnement Toulouse
UMR 5563 CNRS - UR 234 IRD - UM 97 UPS – CNES

Observatoire Midi-Pyrénées
14 avenue Édouard Belin
F-31400 Toulouse
Tél. +33 (0)5 61 33 26 47 - Fax. +33 (0)5 61 33 25 60
www.get.obs-mip.fr

cnes cnrs IRD Institut de Recherche pour le Développement FRANCE UNIVERSITÉ TOULOUSE III PAUL SABATIER Université de Toulouse

Required technical skills:
- Use of ab initio molecular dynamics codes: CP2K, CPMD, CP, PINY-MD. Good level.
- Possibly expertise to build empirical potentials by inverse Monte Carlo approach.
- Possibly experience in path integral molecular dynamics.

Knowledge to put in application:
- Operating molecular dynamics algorithms
- Path integral formulation of quantum mechanics.

Know-how :
- Computer programing : good level
- Developing a scientific approach to set up a methodology aiming at reproducing a quantity measured experimentally.
- Estimating the different sources of error and their consequences on the final result.

Some papers in relation to the proposed work::
Dupuis R., Benoît M, Tuckerman M, Méheut M. (2017), Accounts of chemical research 50 (7), 1597-1605
Méheut M. and Schauble E.S. (2014), Geochimica et Cosmochimica Acta 134, 137-154