

Molecular dynamics simulations of the radionuclide-organic interactions in clay nanopores in the context of geological disposal of radioactive waste

Subatech - Institut Mines-Télécom Atlantique, Nantes, FRANCE

Details of the Ph.D. project

Low permeability Callovo-Oxfordian clay rock is under consideration in France as a possible host rock for long-term disposal of radioactive waste in a deep geological repository. The Callovo-Oxfordian rock serves as an efficient natural geochemical barrier for radionuclides' mobility, but complexation of radionuclides with organic molecules, naturally present in the pore solution or generated by the waste, may significantly affect their adsorption and transport properties. These organic species, such as small carboxylic acids, can be retained by clay through chemical interactions or physical immobilization.

To increase the fundamental molecular scale understanding of the physical and chemical mechanisms controlling the interactions between radionuclides (Cs^+ , Sr^{2+} , UO_2^{2+}), organic molecules, and clay rock, this project is focused on the computational atomistic modeling of the effects of small organic molecules on the adsorption and transport of radionuclides in clay. Clay minerals (phyllosilicates) are inherently layered materials. In addition to the interactions with basal surfaces of clay, the primary focus of the project will be on the interactions with the edges of clay nanoparticles.

Qualifications

The Ph.D. studentship is fully supported in the framework of the *industrial chair "Storage and Disposal of Radioactive Waste"* jointly funded by ANDRA, ORANO, and EDF at the Institut Mines-Télécom Atlantique, Nantes, France.

The successful applicant is expected to have a strong background in physics, chemistry, materials science, or other related field, **a good knowledge of computational chemistry and experience with classical and/or ab initio molecular dynamics calculations**, and a strong interest in the application of these computational molecular modeling techniques to study fundamental atomic-scale properties of technologically, environmentally and geochemically important materials.

The student will work towards a Ph.D. degree in Physics or Chemistry within the joint doctoral school *Molecules, Matter, and Materials* of the Université Bretagne-Loire (the association of 8 establishments of higher education in the regions of Bretagne and Pays de la Loire).

There are no residency or nationality restrictions. Knowledge of French language is not required, but a reasonable level of oral and written command of English is expected.

To apply, please send a detailed CV and the names and addresses of three references to Prof. Andrey G. Kalinichev (kalinich@subatech.in2p3.fr).

For more information about IMTA, Subatech, and our group's recent research projects and publications please visit our web sites at

<https://www.imt-atlantique.fr/en/person/andrey-kalinichev#edit-group-projets-de-recherche>

<http://www-subatech.in2p3.fr/fr/recherche/equipes/radiochimie/recherche/modelisation-moleculaire>