Postdoctoral Position in Computational Molecular Modeling of Cement Materials for Nuclear Waste Disposal Applications

A postdoctoral position is available immediately at the SUBATECH Laboratory (Ecole des Mines de Nantes, FRANCE) in the recently formed research group focusing on the computational molecular modeling of materials and processes relevant to nuclear waste disposal applications. The objective of this particular project is to quantify on the molecular level the effects of organic additives on the adsorption and mobility of nuclear waste species at the surfaces and in the pore water of cement phases (see a detailed description below). The successful applicant should have an earned Ph.D., demonstrated experience with classical and/or quantum molecular computer simulations, and a strong interest in the application of these computational techniques to study the properties of cement and other environmentally and technologically important materials.

Experience with large scale molecular simulations and high performance computing is expected. For more information about our current research activities and publications please visit http://www.emn.fr/z-subatech/kalinich/.

This position is presently funded by ANDRA (Agence Nationale pour la gestion des Déchets Radioactifs) for the period of 18 months.

To apply, please send a detailed CV, a list of publications, and the names and addresses of at least three references to Dr. Andrey Kalinichev (kalinich@subatech.in2p3.fr).

Description of the project

In the process of nuclear waste storage, cementitious materials would be used as the confinement matrix (some FA-MA/VL waste) or in construction work (gallery, sockets, plugs). The development of these materials includes the application of organic polymers at low concentrations (≈ 0.5 to 1% by weight). These polymers (additives) are used for their dispersing properties which prevent the aggregation of cement particles during the hydration process. Furthermore, their addition as superplasticizers (or water-reducers) affects very significantly many fundamental material properties (maturation behavior at the early stage, durability, long-term mechanical properties, etc.).

Given the large volume of concrete used for nuclear waste storage, the evaluation of the effects of polymers on the retention properties of cementitious materials with respect to radionuclides (RN) has already been investigated earlier. The results obtained show that their impact is limited for fresh cement, but no information is available concerning the polymer release as a function of the cementitious degradation. Moreover, given the analytical limitations, no study has been able to propose a quantitative model to predict the residual concentration of additives in the cement pore water and thus to evaluate the influence of these additives on the complexation reactions with the RN and/or competing reactions towards the sorption sites with other molecules from organic waste.

The objective of this postdoctoral project is to quantitatively address these important questions on a fundamental molecular level by applying computational molecular modeling techniques. The processes of organic and radionuclide adsorption at the surfaces of cement particles (calcium silicate hydrates, CSH with different C/S ratio) will be quantitatively assessed using classical and *ab initio* molecular dynamics techniques. Potentials of mean force will be calculated to quantify the structural and energetic characteristics of interactions in the systems organics-RN-cement. This will allow us to better understand and interpret on the fundamental atomistic level the results of experimental measurements and will help to better focus and direct future experimental efforts. This project will also be closely linked with other computational molecular modeling efforts already on-going at the Ecole des Mines de Nantes and Subatech in the context of the industrial chair *"Storage and Disposal of Radioactive Waste"* supported by ANDRA, Areva, and EDF.