Postdoctoral position at IRSN (Cadarache/France):

Quantification of the uncertainties induced by using semi empirical potentials: application to Zirconium hydrides

1) Context and scientific problem

This post-doctoral position is proposed in the framework of the development of multi-scale modeling approaches and their application in the field of materials for energy and environment technological applications. It aims at answering the fundamental question: how and how accurately the important macroscopic characteristics of a technological material can be predicted from interatomic potentials. To quantify the uncertainties, we propose to set up a new methodology, based on the critical analysis of existing experimental and theoretical data, and on the use of efficient approaches in mathematics and data sciences.

This methodology will be implemented in the case zirconium hydrides, which are of prime importance in the field of nuclear energy. Indeed, the cladding of nuclear fuel rods, made of zirconium alloys, are submitted to hydride precipitation which can weaken the rods and limit their lifetime or complicate their transportation and storage. The behavior of these materials and in particular their thermophysical properties result directly from their microstructure, which is driven by the nature of interactions between atoms. These interactions are usually described by simplified energy models with a fixed number of parameters, based on approximations which impact the accuracy of the computed physical data. However, no systematic approach exists up to now to quantify these uncertainties. This failure constitutes a major obstacle to deploying multi-scale approaches to characterize and predict the behavior of complex materials.

2) Goal of the study

The objective of this work is to quantify the uncertainties induced by the use of interatomic potentials, focusing on the case of the Zr-H system. To this aim, powerful statistical approaches will be applied in order to identify the still existing locks. Two main aspects will be explored: first, the impact of the uncertainties associated with the potential parameters on the accuracy of the calculated physical quantities. Then, in a feedback process, and thanks to a sensitivity study associated with these parameters, the identification of actions to be taken to improve their adjustment upstream. This work should lead to the identification of reliable guidelines to optimize the development of controlled potentials.

3) Applicant Profile

The candidate should have a PhD in applied mathematics, in the field of statistics and/or probability, or in Materials science with a strong expertise in uncertainty quantification and programming. She/he must be open-minded towards the field of materials science, and able to interact with the modeling and experimental researchers on this field.

4) Research group

The research will be performed in collaboration with F. Ribeiro and J. Baccou at IRSN (Cadarache), J.-C. Crivello and J.-M. Joubert at ICMPE (Thiais), and G. Tréglia and C. Varvenne at CINaM (Marseille) laboratories. Travels and stays are expected between the three sites.

Applicants should send a cover letter with a detailed CV and two reference contact persons to: fabienne.ribeiro@irsn.fr
The position will start as soon as possible for the selected applicant, and not later than the last quarter of 2019.