Exploration of the energy landscape for atomic diffusion in complex systems

Multi-scale modeling is a strategic tool to understand, optimize and design new materials with improved performance in many industry domains, from aeronautics to pharmacology, including microelectronics. If its efficiency in guiding researchers and engineers is well recognized, the related human cost remains too important to allow a systematic use of computational approaches. The current challenge is therefore to propose efficient, adaptive, and predictive calculation tools, based on atomic granularity while allowing access to materials macroscopic properties.

At this level, the main issue deals with the exhaustive exploration of the energy landscape, *ie* the identification of the atomic events that need to be considered in higher scale models. The different local atomic configurations and the associated energy barriers must be identified by ab initio approaches, like DFT approaches, which requires a huge human investment that is not adapted to material engineering. Several methodologies exist to build this event library, but all of them are expensive in terms of resources and computation time. We propose in this thesis to use a methodology developed at LAAS-CNRS, the Static Modes approach, which allows a systematic and low cost exploration of atomic displacements and their induced effects.

The objective of this thesis is to adapt and couple the Static Modes (MS) algorithm with DFT calculations to guide them and to reduce the intervention of the user, which is necessary until now to provide the exhaustive list of events used to feed other codes, such as Kinetic Monte Carlo. The MS method was initially developed to address biomolecule movements and the complexity of their energy landscapes. We propose to make this methodology transferable to all types of materials of interest (bio-hybrid and inorganic). This new approach must therefore save time in exploring the energy landscape by guiding the DFT and optimizing the choice of significant events for the evolution of the system, and therefore participating in the design of a multi-methodological approach: innovative, predictive scale, adapted to complex systems while maintaining a reduced calculation time.

Application: We are looking for a motivated candidate with a solid background in physico-chemistry and atomic-scale simulation. Good programming skills and DFT tools are also expected.

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