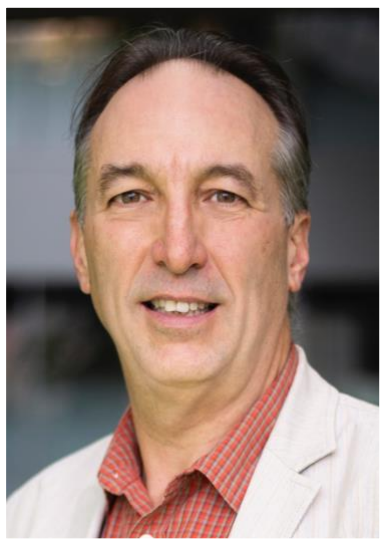
THE DR. AND MRS. SATTI PADDI AND PARVATI REDDY RESEARCH LECTURE

Understanding How Atoms Move in Materials

Wednesday
March 22, 2023

1 p.m. in C-2045
Chemistry-Physics Building



Understanding processes underlying the evolution of materials (aging, defect formation, chemical reactions, and catalysis) requires a precise description of atomic interactions in complex environments and on time scales that exceed, sometimes by a lot, the nanosecond. Faced with these challenges, modellers have long been forced to choose between precision, with heavy quantum computations, and time scale, with much lighter empirical potentials, but that are unable to truly describe the complexity of chemical environments. Even with these more than approximate potentials, traditional simulation methods, such as molecular dynamics, do not allow us to exceed the microsecond, considerably limiting the relevance of models to understand experimental phenomena. A more efficient coupling of accelerated dynamics approaches, such as kinetic ART, an off-grid kinetic Monte Carlo algorithm, with ab initio approaches and potentials developed by machine learning, gives hope that it will soon be possible to remove many of these barriers. In this seminar, Dr. Mousseau will present an overview of the recent developments he is currently pursuing around these methods.

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