Center for the Computational Design of Functional Layered

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Understanding Hydration, One Water Molecule at the Time

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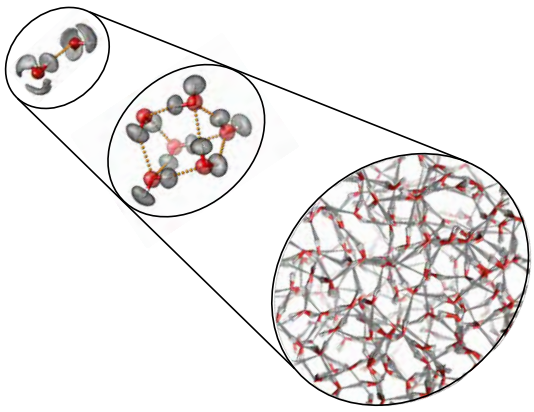

Two of the most challenging problems at the intersection of electronic structure theory and molecular dynamics simulations are the accurate representation of intermolecular interactions and the development of reduced-scaling algorithms applicable to large systems. To some extent, these two problems are antithetical, since the accurate calculation of non-covalent interactions typically requires correlated, post-Hartree-Fock methods whose computational scaling with respect to system size precludes the application of these methods to large systems. I will describe our many-body molecular dynamics (MB-MD) methodology for aqueous systems that overcomes these limitations and enables computer simulations from the gas to the condensed phase, with chemical and spectroscopic accuracy. MB-MD is a unified molecular dynamics framework that combines many-body representations for potential energy, dipole moment, and polarizability surfaces, derived entirely from correlated electronic structure data using supervised learning techniques, with quantum dynamics methods that explicitly account for nuclear quantum effects. The accuracy of the MB-MD methodology is assessed through the analysis of several properties of aqueous systems across different phases with a particular focus on nuclear quantum effects and vibrational spectra.

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Francesco Paesani received his M.S. in Chemistry (1996) and Ph.D. in Theoretical Physical Chemistry (2000) from the University of Rome ''La Sapienza'' (Italy). During his graduate studies, he worked on the extension of density functional theory (DFT) to the treatment of van der Waals interactions and developed the first version of the DFT+DISP approach, which was later popularized as DFT-D, to study weakly interacting systems. After graduation, Francesco joined the group of Prof. Whaley (University of California, Berkeley) as a postdoctoral fellow to study quantum fluids, with a specific focus on the emergence of superfluidity in He^4 and H_2 clusters. He then moved for a second postdoc to the group of Prof. Greg Voth (University of Utah) to work on the development of new methods to model quantum dynamics in condensed-phase systems. In 2009 Francesco joined the Faculty of the Department of Chemistry and Biochemistry at the University of California, San Diego, where is currently an Associate Professor. His group research focuses on the development, implementation, and application of new theoretical and computational methodologies at the intersection of chemistry, physics, and computer science for molecular simulations of aqueous systems and porous materials, with chemical and spectroscopic accuracy. Francesco received the OpenEye Outstanding Junior Faculty Award from the American Chemical Society in 2014, the CAREER Award from the National Science Foundation in 2015, and the Early Career Award in Theoretical Chemistry from the American Chemical Society in 2016.