Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments

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Overview

This project combines expertise from academe and National Labs to advance the state of ab initio molecular dynamics (AIMD) simulation in handling hydrated ions in situations relevant for future research applications dealing with energy and the environment. To do so, community AIMD codes will be elaborated and augmented to incorporate new theoretical concepts and recent algorithmic advances, and to run more efficiently on the DOE Leadership Class computing platforms. This project complements the on-going experimental effort at the DOE Labs to probe the microscopic structure of water solutions using advanced spectroscopic techniques. Building the capacity of predicting from basic quantum theory ionic processes and spectroscopic observations in solution is a grand-challenge for Materials and Chemical Sciences that will be addressed by our interdisciplinary team.

The major goals of the project are:

- Develop and implement a novel path integral (PI) AIMD methodology for water and aqueous media using an advanced *nonlocal* density functional that includes van der Waals interactions and minimizes the self-interaction error.
- Develop and implement an efficient many-body methodology to compute core and valence electron excitation spectra for disordered materials.
- Apply the above methodologies to state-of-the-art simulation studies of the most important aqua ions to elucidate the role of charge transfer interactions in biological environments and the role of water in contact with nanostructured

materials.

- Develop a new computational methodology (Pole Expansion plus Selected Inversion) for solving the Kohn-Sham problem with optimal size scaling properties and combine it with PI-AIMD to enable AIMD simulations of aqueous systems of unprecedented size, as this has the potential of boosting applications to biology and nanotechnology.

To achieve these goals major challenges will be addressed, involving (a) *physics and chemistry theory*, to devise accurate and computationally efficient approaches for electron correlation; (b) *numerical simulation*, to implement new sampling and time evolution approaches that include nuclear quantum effects; (c) *applied mathematics*, as algorithms with optimal scaling properties are needed for large and disordered systems; (d) *computer science*, to design algorithms that exploit the multi-/many-core nodes and the massive parallelism of the most advanced compute platforms; (e) *visualization and data analysis*, to develop new tools to deal with the large amount of data generated in quantum simulations.