

Computational Molecular Modeling of Aqueous Interfaces for Environmental and Materials Science Applications

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Molecular-level knowledge of the thermodynamic, structural, and transport properties of nano-confined water and aqueous interfaces with various materials is crucial for quantitative understanding and prediction of many natural and industrial processes, including mineral weathering, geological carbon sequestration, water desalination, geological nuclear waste storage, cement chemistry, fuel cell technology, etc. Computational molecular modeling is capable of significantly complementing the experimental investigations of such systems and can provide invaluable atomic-scale picture of the materials and processes involved, leading to a greatly improved understanding of the specific effects of the substrate structure and composition on the structure, dynamics and reactivity of the interfacial and nano-confined aqueous solutions.

However, atomic-scale simulations are often quite challenging for many of such systems (clays, cementitious materials, etc.), because their crystal structure and atomic composition are usually not well defined and often characterized by a significant degree of structural and compositional disorder. ClayFF was originally developed in response to a strong need for a robust and flexible force field for classical molecular simulations of such interfaces and their interactions with organic and bio- molecules in aqueous environment [1]. This talk will provide a brief overview of the fundamental assumptions and limitations of the ClayFF approach to the atomistic modeling of these complex systems, focusing on the most recent MD simulation results on clay-related and cement-related materials, and on the most recent improvements of the original ClayFF parameterization for better agreement with experiments [2-4].

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