Molecular Dynamics and Quantum Chemistry Studies of Complex Soil Organic Matter Interactions with Solvated Metal Ions and Mineral Surfaces

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Mineral surfaces can potentially physically protect soil organic matter (SOM) against decomposition and ultimate mineralization to small molecules which can provide nutrients for plants and soil microbes and can also contribute to the Earth's elemental cycles. As a complex mixture of organic molecules of biological origin at varying degrees of decomposition, SOM, itself, can self-assemble in such a way as to expose some biomolecule types to biotic and abiotic attack while protecting other biomolecule types. The interplay of van der Waals and electrostatic interactions drive the organization of SOM and SOM with mineral surfaces and solvated metal ions. Here, for the first time, we employ large scale classical atomistic molecular dynamics (MD) simulations to shed light on assemblies of organic molecules alone or in complexation with mineral surfaces and solvated metal ions. In an aqueous solvated environment, we also demonstrate the formation of dissolved organic matter (DOM) that may be carried away from mineral surfaces with water transport. Abiotic chemical reactions are also an important consideration in potential chemical changes of the organic species such as oxidation/reduction and degradation. With structural insight from our MD simulations, quantum chemistry methods can be employed to further investigate the chemical reactivity of SOM and DOM with mineral surfaces and solvated metal ion species. Moreover, spectroscopic signatures based on chemical structure can be simulated by quantum chemistry methods to interpret spectra from x-ray absorption spectroscopy (XAS) and other spectroscopic techniques. In this presentation, we will also discuss our MD and quantum chemistry findings on a model SOM system interacting with mineral surfaces and solvated metal ions.