

# **Understanding Molecular-scale Complexity and Interactions of Soil Organic Matter**

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## **Abstract**

The goal of our proposed research is to focus on the fundamental molecular-level (nanometer) structure and interactions of soil organic matter (SOM) using well-established approaches that provide unparalleled and unique atomistic and molecular information. Specifically, we will combine state-of-the-art molecular modeling approaches with nuclear magnetic resonance (NMR) and X-ray absorption spectroscopic (XAS) techniques. We will focus on characterizing the structure, energetics and spectroscopic signatures of model humic substances (HSs) and precursor components (biopolymer residues), their interactions with environmentally relevant mineral surfaces (silicates, clays, iron and aluminum oxides) and complexation with ions (involving P, Ca, Fe, K) with an eye to understanding how molecular scale interactions influence the emergent structures and properties on larger scales. EMSL is the ideal catalyst to set this effort in motion as this multi-modal approach, with molecular modeling included, is a largely unexplored area in soil science.