Microscopic analysis of the structure, dynamics, and adsorption properties of the standard Leonardite humic acid using molecular dynamics simulations

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Humic substances (HS) are abundant in the environment and play an important role in a number of biogeochemical processes including microbial activity, soil aggregation, plant growth, retention and release of nutrients, environmental fate of pollutants, and carbon storage. They are flexible, relatively small molecules forming supramolecular structures through intermolecular interactions. Despite the great importance of understanding their behavior at the atomic level, computational modeling, a premier high-resolution technique providing a great level of details, has been surprisingly little employed to study humic substances. In this work, we use the recently developed Vienna-Soil-Organic-Matter Modeler[1] to create representative structural models of a real HS sample, the standard Leonardite humic acid. The strength of adsorption was estimated for a range of small organic compounds in a dry and fully hydrated Leonardite model. Strikingly, our results show a remarkable level of matching with experimental sorption data. Moreover, molecular dynamics simulations were used to probe the structure and dynamics of the system at a range of hydration levels, where the studied systems were characterized in terms of their physical-chemical properties, including density, dielectric properties, hydrogen bonding, etc.

1. A. Sündermann et al., J. Mol. Graph. Model. 62, 253–261 (2015); http://somm.boku.ac.at/