Goldschmidt 2025 Abstract
https://doi.org/10.7185/gold2025.29894

Aggregation of soil constituents to mineral surfaces

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The interfaces between soil minerals and their surroundings serve as a basis where nutrients and contaminants tend to aggregate. The properties of the interface depend on several factors such as the mineral particle size, exposed mineral surfaces, the available soil organic matter (SOM) and its chemical nature, water content, soluble cations and their concentrations, and the electrostatic properties of the surrounding environment.

During the last decades, several atomistic models have been proposed as an approximation for the behavior of soil at the microscopic level. With the arise of new models, such as the Vienna Soil-Organic-Matter Modeler (VSOMM), the chemical diversity and structure of SOM is a novel factor to consider.

In this work, we generated different models of humic substances using the VSOMM and modeled their interaction with Kaolinite, one of the most abundant clay mineral found in soils. Our results exhibit the contribution of key components on the organo-mineral interfaces which ultimately explain the adsorption process.

References:

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