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Molecular-Scale Unveiling of Diverse Organic Binding Modes with Clays and Iron Oxyhydroxide Minerals by Combining Molecular Modeling Simulations with Experimental Spectroscopic Data

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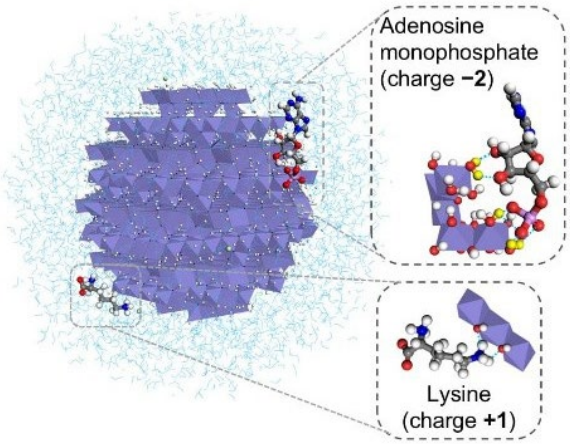

Organic matter associations with minerals in soils and sediments are critical to the residence time of organic matter in environmental matrices,[1,2] by influencing trapping, turnover, and transport rates. Clays and iron oxyhydroxides are amongst important mineral types predominantly found in mineral-organic associations. As observed in field and laboratory studies, these associations can involve organic matter of various structures and charges. However, the molecular-scale interactions that drive unexpected binding affinities have remained mostly hypotheses. Through the combination of molecular modeling simulations with multiple spectroscopic data, my team has sought to obtain evidence for different types of proposed interactions. We have performed adsorption experiments of different types of biomolecules (sugars, amino acids, ribonucleotides, lignin-derived phenolic acids), reacted with montmorillonite (as a smectite clay) or ferrihydrite (as an iron oxyhydroxide).[3,4] The interactions in the mineral-organic complexes are examined through Fourier transform infrared spectroscopy[4] and X-ray diffraction[3] (in the reaction with the clay). For three-dimensional views of the adsorbate conformations responsible for identified interactions, we have employed molecular dynamics simulations coupled with quantum mechanics-determined transition state structures and quantum mechanics-calculated binding energies. Taken collectively, the coupling of experimental and theoretical techniques has afforded new insights on diverse types of organic binding during adsorption of organic matter on clays and iron oxyhydroxides. These insights contribute to predictive understanding on the role of minerals in the geochemical fate of organic matter.

References: 1. Hemingway, J. D.; Rothman, D. H.; Grant, K. E.; Rosengard, S. Z.; Eglinton, T. I.; Derry, L. A.; Galy, V. V. (2019) Mineral protection regulates long-term global preservation of natural organic carbon. **2.** Georgiou, K.; Jackson, R. B.; Vinduskova, O.; Abramoff, R. Z.; Ahlstrom, A.; Feng, W. T.; Harden, J. W.; Pellegrini, A. F. A.; Polley, H.W.; Soong, J. L.; et al. Global stocks and capacity of mineral-associated soil organic carbon. **3.** Wang J., Barrios-Cerda B., Aristilde L. (2025) Surface charge heterogeneity and mechanisms of organic binding modes on an iron oxyhydroxide. **4.** Wang J., Wilson R.S., Aristilde L. (2024) Electrostatic coupling and water bridging in adsorption hierarchy of biomolecules at water-clay interfaces, Proc. Nat. Acad. Sci., 121 (7), e231656912.