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REVIEW

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NMR and computational molecular modeling studies of mineral surfaces and interlayer galleries: A review

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ABSTRACT

This paper reviews experimental nuclear magnetic resonance (NMR) and computational molecular dynamics (MD) investigations of the structural and dynamical behavior of cations, anions, H_2O, and CO_2 on the surfaces and in the interlayer galleries of layer-structure minerals and their composites with polymers and natural organic matter (NOM). The interaction among mineral surfaces, charge-balancing cations or anions, H_2O, CO_2, and NOM are dominated by Coulombic, H-bond, and van der Waals interactions leading to statically and dynamically disordered systems and molecular-scale processes with characteristic room-temperature frequencies varying from at least as small as 10^2 to $>10^{12}$ Hz. NMR spectroscopy provides local structural information about such systems through the chemical shift and quadrupolar interactions and dynamical information at frequencies from the sub-kilohertz to gigahertz ranges through the T_1 and T_2 relaxation rates and line shape analysis. It is often difficult to associate a specific structure or dynamical process to a given NMR observation, however, and computational molecular modeling is often effective in providing a much more detailed picture in this regard. The examples discussed here illustrate these capabilities of combining experimental NMR and computational modeling in mineralogically and geochemically important systems, including clay minerals and layered double hydroxides.

Keywords: Mineral surfaces, mineral-fluid interactions, clay minerals, natural organic matter, NMR, molecular dynamics, computational modeling, layered double hydroxides, Review article, Invited Centennial article