# Structural Complexity in the Fate of Pharmaceuticals at Water-Mineral Interfaces: Computational and Spectroscopic Investigations

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Expanding clay minerals such as smectites can form interlayer nanopores that traps organic molecules in mineral particles suspended in surface waters, embedded in lake and river sediments. Elucidating the underlying mechanisms is important for understanding the role of these minerals in the fate of polar organic contaminants including pharmaceuticals. Retention of these contaminants within smectite clay minerals have been attributed primarily to cation exchange. However, spectroscopic investigations are highlighting that other mechanisms deserve further consideration in characterizing the adsorption mechanisms to smectite-type clay minerals under different environmental conditions. The activities of my research group have applied a combination of spectroscopic experiments and molecular modeling simulations to obtain a comprehensive mechanistic account of pharmaceutical-clay interactions as a function of pH and presence of multivalent cations. Our research efforts have focused on tetracycline and fluoroquinolone antibiotics. Adsorbate interactions and structures were evaluated using X-ray diffraction (XRD), infrared (IR), and solid-state nuclear magnetic resonance (NMR) spectroscopies, complemented with molecular dynamics simulations. Our findings stress the important role of adsorbate structures influenced by both pH and metal cations in facilitating favorable polar contaminant-smectite clay complexes that are beyond cation exchange-type mechanisms.
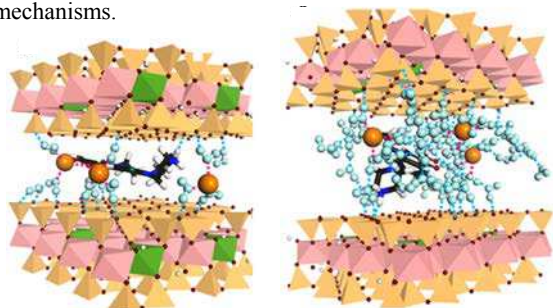
Figure 1. Molecular dynamics-optimized structures of ciprofloxacin (left) and moxifloxacin (right) adsorbed in the interlayers of montmorillonite, a smectite clay mineral.

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