

Eawag Seminar Invitation

Structural Complexity in the Fate and Trapping of Pharmaceuticals and Cyanotoxins at Water-Mineral Interfaces

Speaker **Dr. Ludmilla Aristilde**

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When **March 2, 11.00 – 12.00 a.m.**

Where **Forum Chriesbach, room C20, Eawag Dübendorf**

Abstract Expanding clay minerals including smectites can form interlayer nanopores that traps organic molecules in mineral particles suspended in surface waters or 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. 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 contaminant-clay interactions as a function of pH and presence of multivalent cations. Our research efforts have focused on tetracycline and fluoroquinolone antibiotics as well as cyanobacterial toxins. 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 contaminant-smectite clay interactions that are beyond cation exchange-type mechanisms.