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From Bulk to Nanopore: Exploring the Physicochemical Causes of Unconventional Behavior of Confined Water in Mineral Systems

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Confined water is ubiquitous in nature, and research indicates that water confined within mineral nanopores undergoes significant changes in its thermodynamic and dielectric properties, and chemical activity compared to its bulk counterpart. In a natural system, this manifests as substantial mechanical and chemical alterations to mineral properties such as complexation, mineralization, and dissolution. However, the underlying interfacial molecular mechanisms governing these changes are poorly understood.

This presentation will offer evidence of water's unconventional behavior, such as changes in mobility on mineral surfaces and inside mineral nanopores, and will explore the underlying physicochemical causes. A central question is the role of interfacial chemistry in modifying water behavior and driving the observed confinement effects.

In complex natural environments involving gases and organic matter, this process becomes even more challenging to study. We will first discuss prior research on the dynamic nature of calcite surfaces in humid air. Subsequently, we will detail observations of chemical dynamics at the nanometer scale on mineral surfaces using near-field infrared (IR) spectroscopy. Additionally, we also employ nuclear magnetic resonance (NMR) spectroscopy to directly measure the mobility of water within naturally occurring mineral nanotubes and in the confined phases between single-crystalline natural calcite surfaces. Finally, we use molecular dynamic simulations to explain these experimental observations.