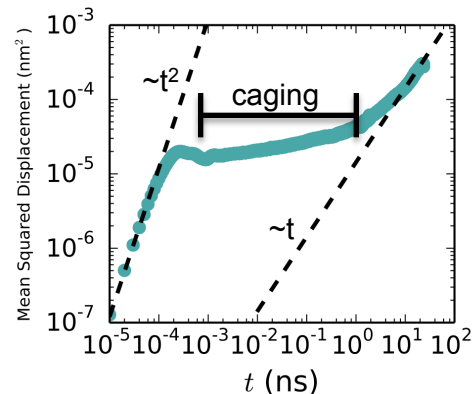
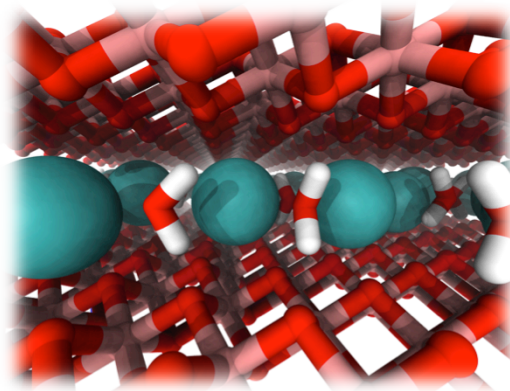




Michael L. Klein

# Multi-Scale Modeling of Catalytic Interfaces



Strong interactions between MnO<sub>2</sub> (red/pink), water (red/white), and K<sup>+</sup> (green) lead to slow, collective dynamics in the confined interlayer region.

## Keys features

- Computer Simulations
- Model Development
- Water Splitting

## Scope of effort

- Interaction of water with pristine surfaces and surface defects; collaborative effort with Umesh Waghmare (JNCASR)
- Properties of heterophase interfaces across scales
- Design strategies for efficient photocatalytic materials

## Challenges to address

- Develop interaction potentials that capture the rich structure and thermodynamic properties of layered materials and their interfaces
- Describe the reactivity of water at the surface of novel photocatalysts



Umesh V. Waghmare