Multi-Scale Modeling of Catalytic Interfaces

**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