



John Pederson

Joslin/Mary Jo Peed Award
Ph.D. Student, Chemistry
First Year ARCS Scholar

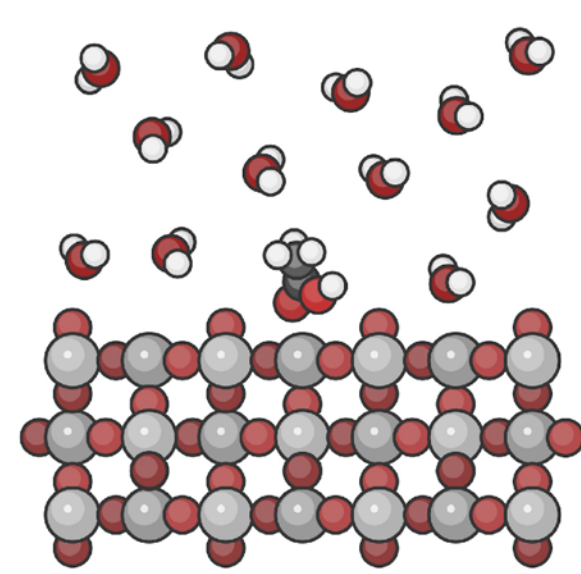
Georgia Tech



Multi-scale Modeling of Chemistry at Solid/Liquid Interfaces

Hybrid quantum mechanical/molecular mechanics (QM/MM) allows us to model reacting systems with quantum chemical accuracy while efficiently including the influence of complex environments.

Heterogeneous Catalysis



TiO₂(110)/Aqueous Interface

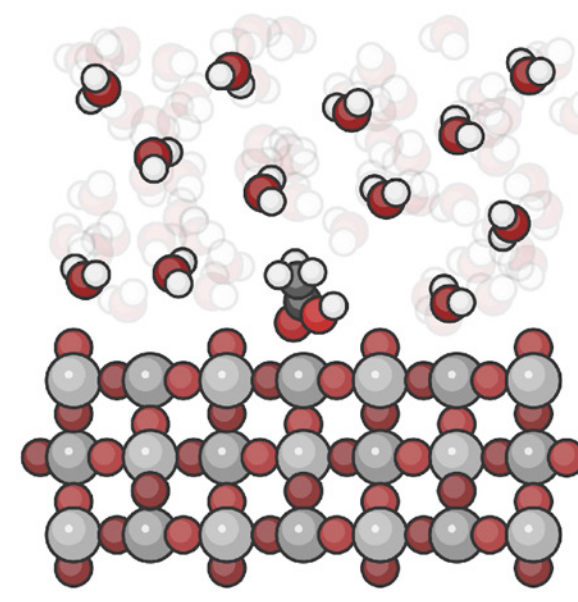
Catalysis at S/L Interface

- No thermal decomposition
- Larger substrates
- Complex reaction pathways

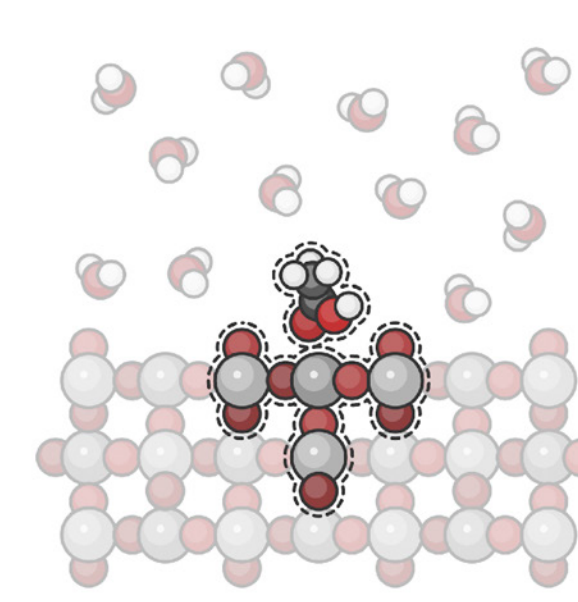
Model Surface: Rutile TiO₂

- Biomass refining
- Photocatalysis
- Catalyst support

Modeling Challenges



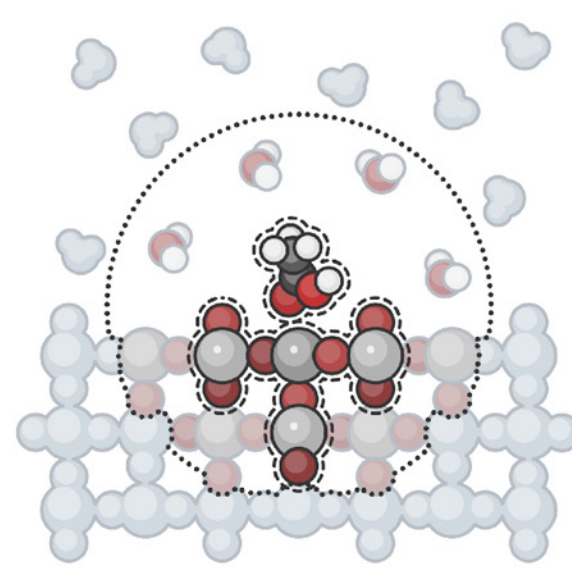
Configuration Sampling



Large Systems

← Computationally Expensive →

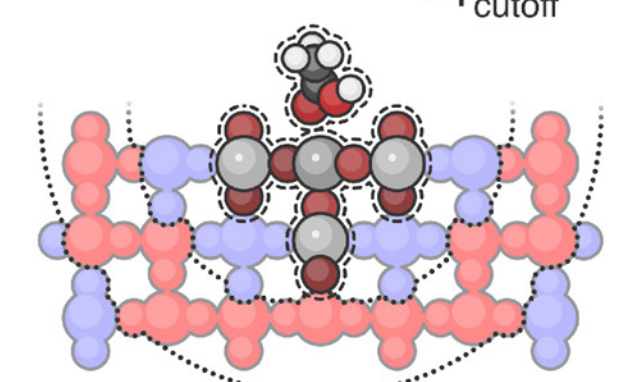
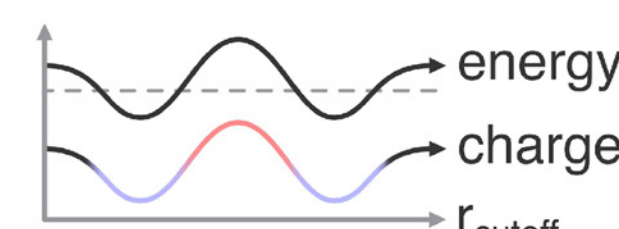
Multiscale Approach



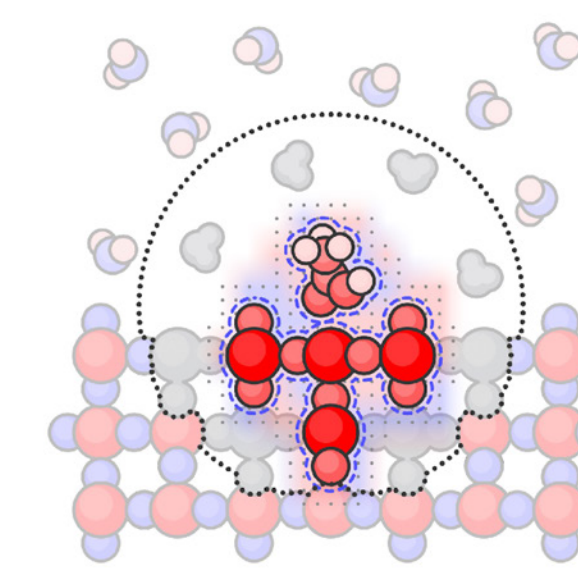
Quantum Mechanics/
Molecular Mechanics

- Region I nuclei
 - Region I electrons
 - Region II atoms
 - Region III atoms
 - Region II/III boundary
- QM
- MM

Long-Range Electrostatics

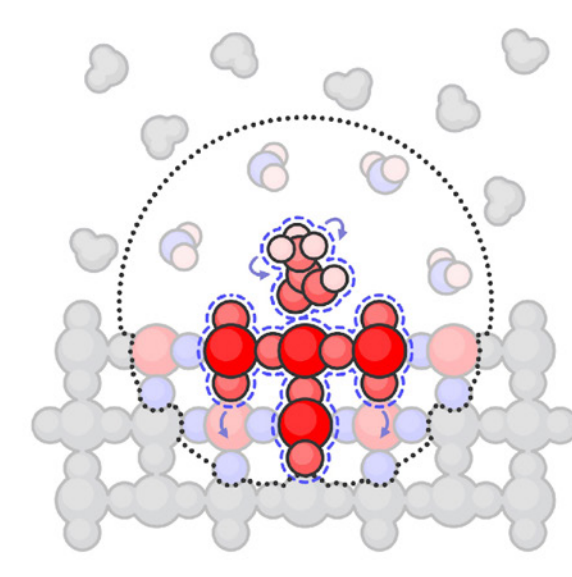


charge [e]

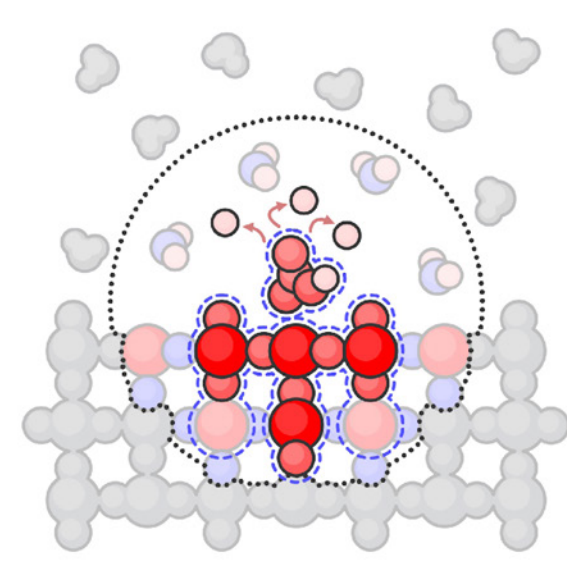


Gridpoints with Region III electrostatic potential

Close-Range Electrostatics

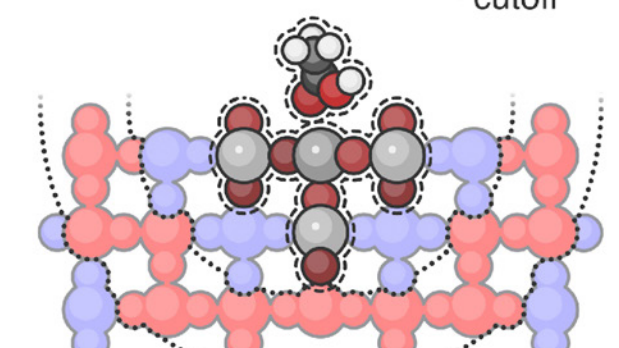
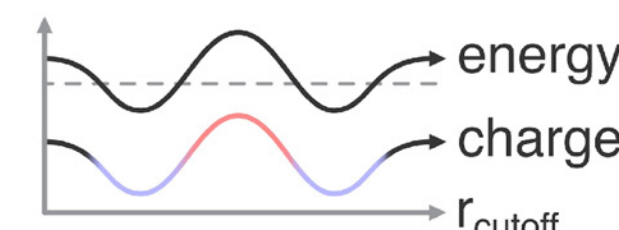


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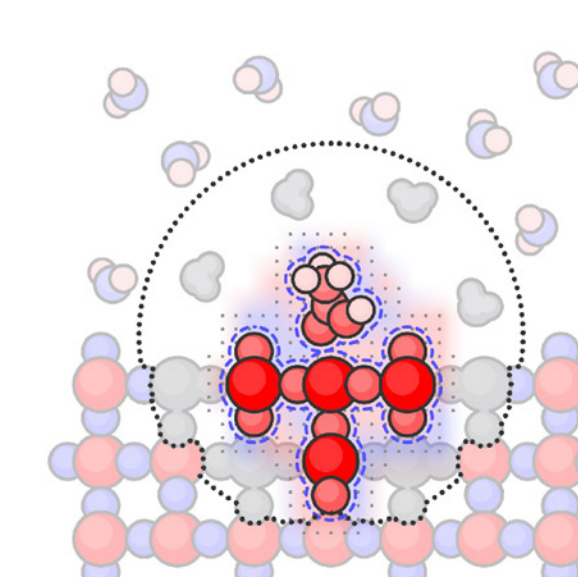


Electrons "spill-out"
onto nearby (+) charges

Long-Range Electrostatics



charge [e]



Gridpoints with Region III electrostatic potential

Scholar Awards Celebration

November 13, 2024



Igniting
Innovation
in Georgia