John Pederson

Mary Jo Peed/Joslin Award

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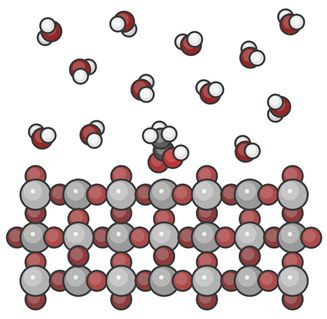
Multi-scale modeling of chemistry at solid/liquid interfaces

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



TiO_2(110)/Aqueous Interface

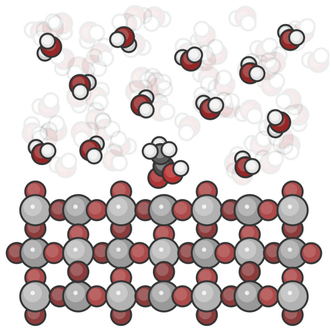
Catalysis at S/L Interface

- No thermal decomposition
- Larger substrates
- Complex reaction pathways

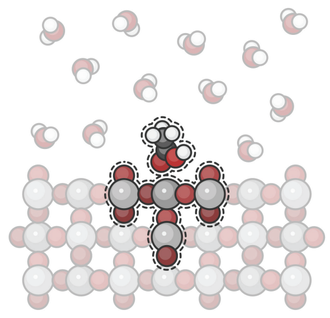
Model Surface: Rutile TiO_2

- Biomass refining
- Photocatalysis
- Catalyst support

Modeling Challenges



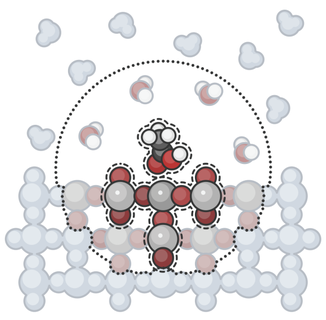
Configuration Sampling



Large Systems

Computationally Expensive

Multiscale Approach



Quantum Mechanics/ Molecular Mechanics

- Region I nuclei
- Region I electrons

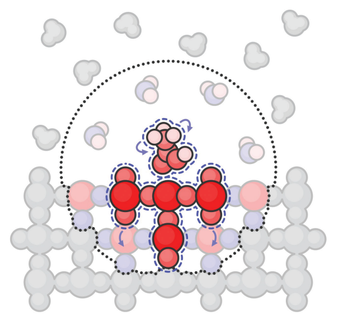
QM

- Region II atoms
- Region III atoms

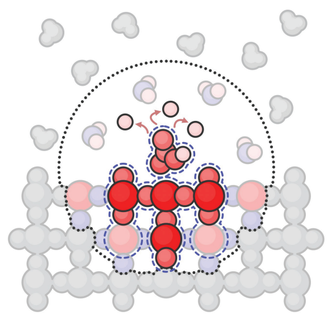
MM

- Region II/III boundary

Close-Range Electrostatics

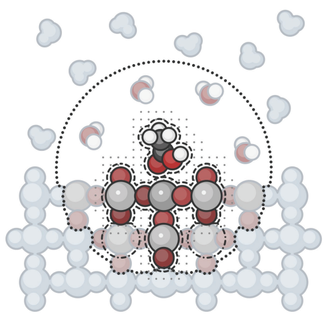


charge [e]



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

Pseudopotential Approach



- Region II pseudopotential

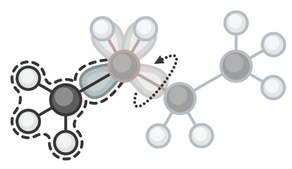
Advantages

- Simple implementation

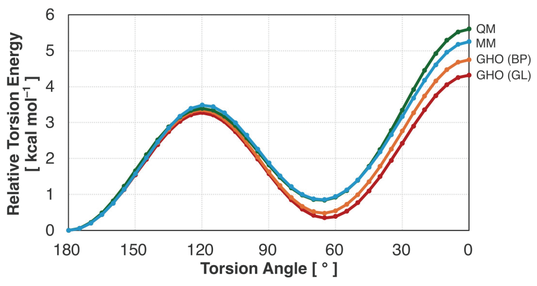
Disadvantages

- Requires integer formal charges instead of more accurate partial charges
- Pseudopotentials are not readily generalized

Generalized Hybrid Orbital Approach



- Boundary atom
- Active hybrid orbital
- Auxiliary hybrid orbital



Next Steps

- Extend GHO approach to model the TiO_2 surface

Scholar Awards Celebration

November 12, 2025

SCHOLAR AWARDS CELEBRATION ARCS FOUNDATION ATLANTA

Igniting Innovation in Georgia