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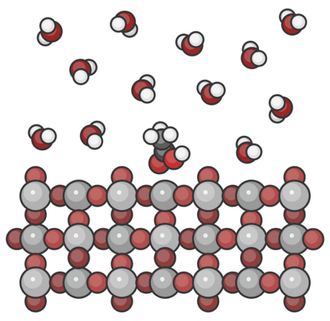
Multi-scale modeling of chemistry at solid/liquid interfaces

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

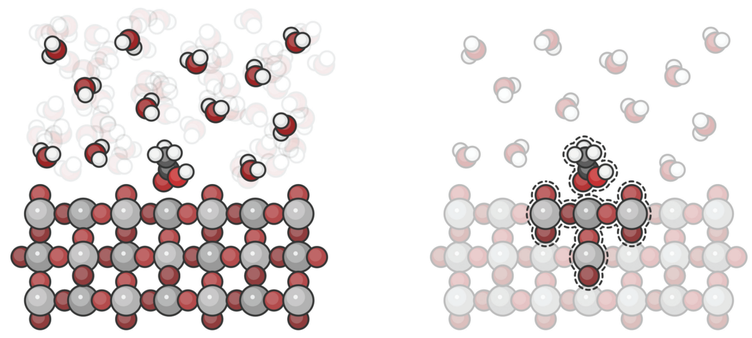
Catalysis at S/L Interface

- No thermal decomposition
- Larger substrates
- Complex reaction pathways

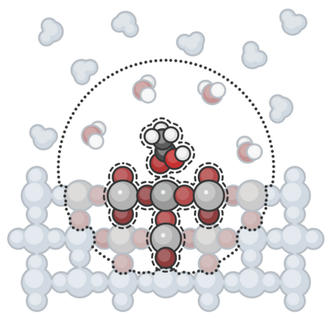
Applications

- Biomass refining
- Photocatalysis
- Catalyst support

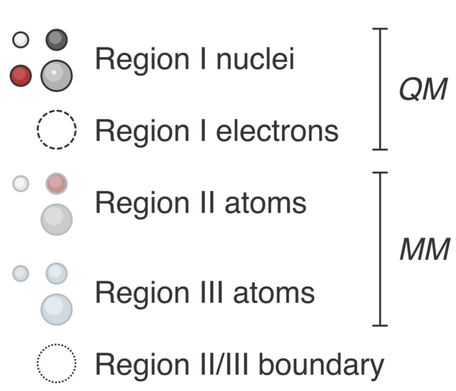
Modeling Challenges



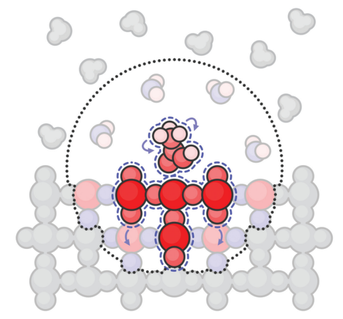
Multiscale Approach



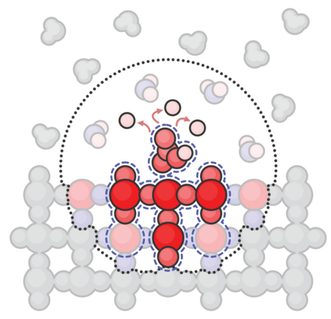
Quantum Mechanics/ Molecular Mechanics



Close-Range Electrostatics



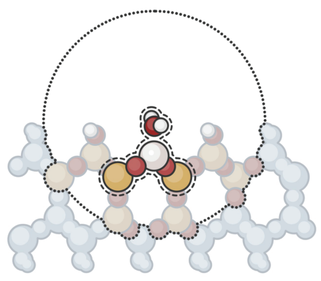
Electrons "spill-out" onto nearby (+) charges



Generalized Hybrid Orbital Approach

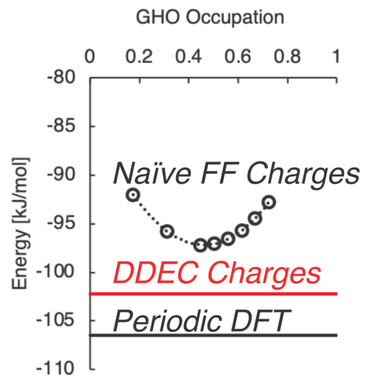


Test System



β-SiO_2 w/ Al Defect

Generalized Hybrid Orbital Benchmarks



Verification Benchmark

- Compared against periodic DFT (VASP)
- Level of agreement depends on quality of charges:
  - < 10 kJ/mol for FF
  - < 5 kJ/mol for DDEC
- GHO is ~20x faster than Periodic DFT

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