

Ab initio Multi-Scale Modeling

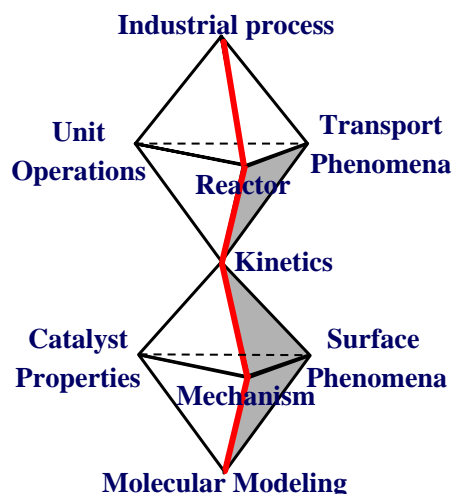
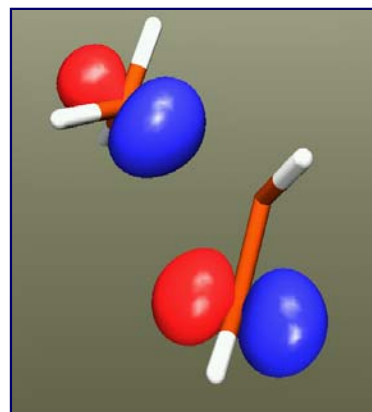
A New Tool for the Sustainable Development of
Chemical & Biological Processes

Complex Radical Chemistry

Non-empirical predictive kinetic models for complex gas phase chemistry involving thousands of reactions are developed from the first principles of physics.

Ongoing Projects

- On-the-fly Prediction of Kinetic Parameters
- Steam Cracking: from Molecules to Industrial Processes
- Non-empirical Models for Atmospheric Chemistry
- Computer Aided Reaction Network generation



Catalytic Reaction Engineering

Simulations provide molecular level insight into catalytic processes, providing leads for the design of selective catalysts.

Ongoing Projects

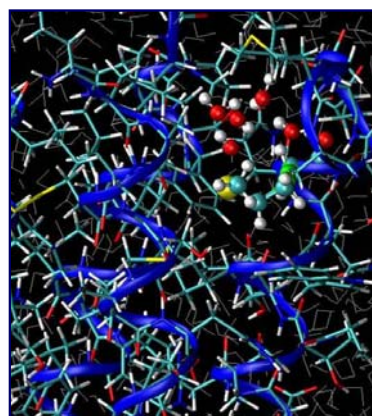
- Catalyst Design for Partial Oxidation
- Aromatics Hydrogenation for Cleaner Fuels
- *Ab initio* Reaction Path Analysis

Novel Materials and Processes

Molecular modeling is used to elucidate and optimize novel biochemical, environmental and nano-electronic processes and materials.

Ongoing Projects

- Process Design for Protein Crystallization
- Molecular Electronics
- Environmental Chemistry of Iron Hydroxides



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