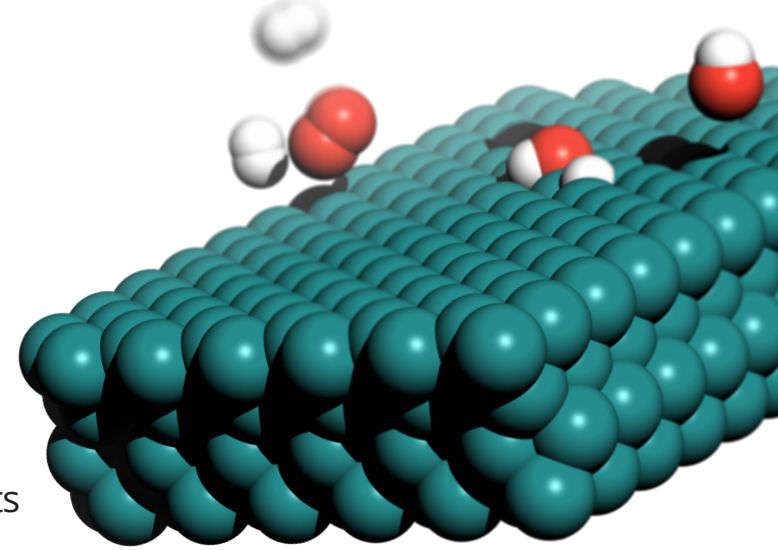
Accelerate the design of high-performance heterogeneous catalysts

Efficient computational solutions leveraging atomic-scale simulation, machine learning, and enterprise informatics for catalytic reactions using solid-state catalysts



Key Capabilities for Catalyst Design

- Gain insights into catalyst performance targets
  - Activity and selectivity
  - Stability and poisoning
- Elucidate reaction mechanisms and active sites
- Calculate activation energies, heats of reactions and reaction rates
- Evaluate surface phase diagrams via combinatorial enumeration
- Elucidate diffusion mechanisms and diffusion constants for diffusion limited processes
- Leverage materials informatics for catalyst optimization

Intuitive Software, Powerful Workflows

- Generate atomic scale models of reactions at surfaces
- Run high-throughput automated simulation workflows
- Build machine learning models with cheminformatics tools
- Leverage the expertise of Schrödinger's scientific support team

Quickly build your skill set for more impactful catalyst design

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