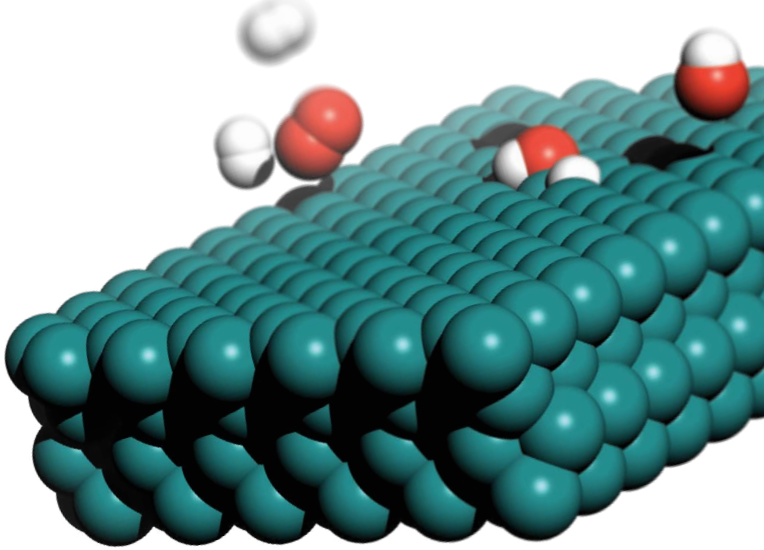
Accelerate the design of high-performance heterogeneous catalysts

Efficient computational solutions leveraging atomic-scale simulation, machine learning, and enterprise informatics



Key capabilities to address R&D challenges

- Gain insights into catalyst performance
  - Activity and selectivity
  - Stability and poisoning
- Identify active sites and elucidate reaction mechanisms
- Calculate activation energies, heats of reactions, and reaction rates
- Evaluate surface phase diagrams via combinatorial enumeration
- Elucidate mechanisms of diffusion-limited processes
- Leverage materials informatics for catalyst optimization
- Apply microkinetic modeling for the analysis of efficiencies and bottlenecks of catalytic processes

Intuitive software with advanced structural builders and workflows

- Generate atomic scale models of surface reaction pathways utilizing structure builders for complex systems
- Run high-throughput automated simulation workflows
- Build machine learning models with cheminformatics tools
- Leverage the expertise of Schrödinger's scientific support team
- Perform user-friendly ab initio molecular dynamics

Quickly build your skill set for more impactful catalyst design

Not familiar with Schrödinger's software? Benefit from vast educational resources, self-paced courses, and 1:1 training tailored for you.

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