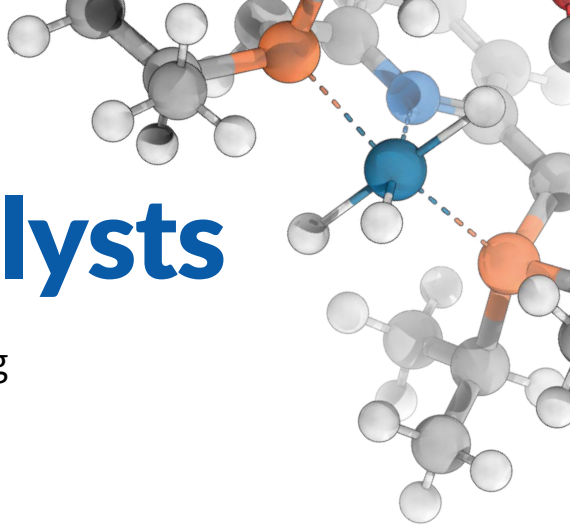
Accelerate the design of high-performance homogeneous catalysts



Efficient, highly-automated solutions for computational molecular design of catalysts leveraging the combination of quantum mechanics, molecular dynamics, and machine learning

Key Capabilities for Catalyst Design

- Direct catalyst design:
  - High turnover frequency catalyst design
  - Enantio-, regio- and chemoselective catalyst design
  - Control over unwanted reaction channels
- Indirect catalyst design:
  - Understand catalytic reaction mechanisms with static and dynamic methods
  - Elucidate mechanisms of chirality generation
  - Gain insights into origin of regio- and chemoselectivity
  - Include conformational effects and calculate ensemble free energy
- Catalyst physical properties:
  - Elucidate structures of organo- and organometallic catalysts
  - Perform conformational space sampling
  - Calculate IR, Raman, UV-Vis and NMR spectra
  - Evaluate thermal decomposition via a single-ended reaction network

Intuitive Software, Powerful Workflows

- Run high-throughput automated simulation workflows
- Save time with Jaguar's unique pseudospectral approximation
- Build machine learning models with automated cheminformatics tools
- Accelerate calculations using extended tight-binding methods
- Leverage the expertise of Schrödinger's scientific support team

Quickly build your skill set for more impactful catalyst design

Not familiar with computational homogeneous catalysis and Schrödinger tools? Benefit from vast educational resources, self-paced courses, and 1-1 training tailored for your area of interest.

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