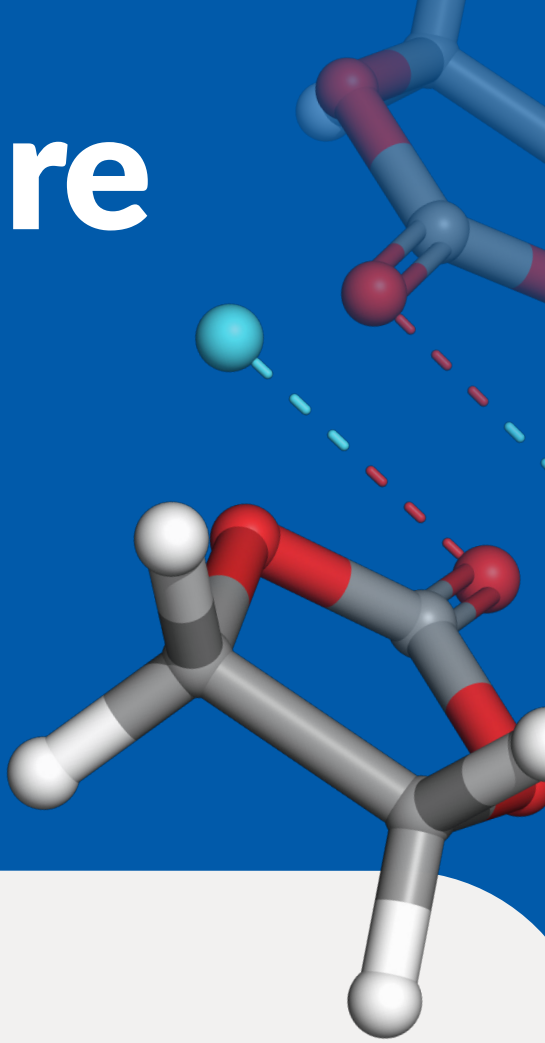
Energy Capture and Storage

Develop the next generation of battery materials that are lighter, safer, more energy-efficient, and cost-effective; Address materials problems in energy capture and storage devices with integrated atomistic simulation tools and workflows; Predict critical properties of component materials and interfaces for batteries, fuel cells, and photovoltaics.



Gain control at the atomic scale

- Utilize advanced atomistic model builders to explore energy materials and interfaces
- Employ physics-based and machine-learning-augmented models to simulate atomic processes, reactions, and materials properties
- Leverage cutting-edge machine learning techniques to find patterns in data

Discover new materials and chemistries

- Accelerate materials discovery and development timelines
- Rapidly screen new material candidates using high-throughput simulation workflows
- Identify novel materials solutions with improved performance

Leverage dedicated professional support

- Engage with Schrödinger experts in energy storage applications
- Benefit from timely and dedicated scientific support

Schrödinger | Materials

Schrödinger's Materials Science Suite provides insights into critical properties for optimized battery design

Cathode/ Anode Properties

- Capacity and ion intercalation potential
- Ion mobility and kinetics
- Structural and chemical stability

Electrolyte Properties

- Electrolyte salt solubility
- Transport properties such as diffusion, ionic conductivity, transference number and viscosity
- Electrochemical stability & reactivity
- Dielectric properties
- Ion solvation and desolvation energetics
- Key properties of functional additives including solubility, viscosity, electrochemical stability window, chemical stability, and reactivity

Electrode-Electrolyte Interfaces

- Electrolyte stability and reactivity towards electrode materials
- Solid electrolyte interphase (SEI) formation reactions and electrolyte degradation mechanisms
- High throughput calculation of electrolyte properties relevant to SEI formation
- Modeling of nucleation and growth of realistic SEI morphologies using template based reactive MD

Contact us: ms-sales@schrodinger.com
Learn more: www.schrodinger.com/materials-science/solutions/energy-capture-and-storage

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Connect with an expert to learn more