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

Discover New Materials and Chemistries

- Accelerate optimized materials discovery and development timelines
- Rapidly screen new material candidates using high-throughput simulation workflows

Generate More Value from Knowledge

- Leverage cutting-edge machine learning techniques to find patterns in data
- Identify novel materials solutions with improved performance
- Engage with Schrödinger experts in energy storage applications

Schrödinger | Materials

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

Cathode/Anode Properties

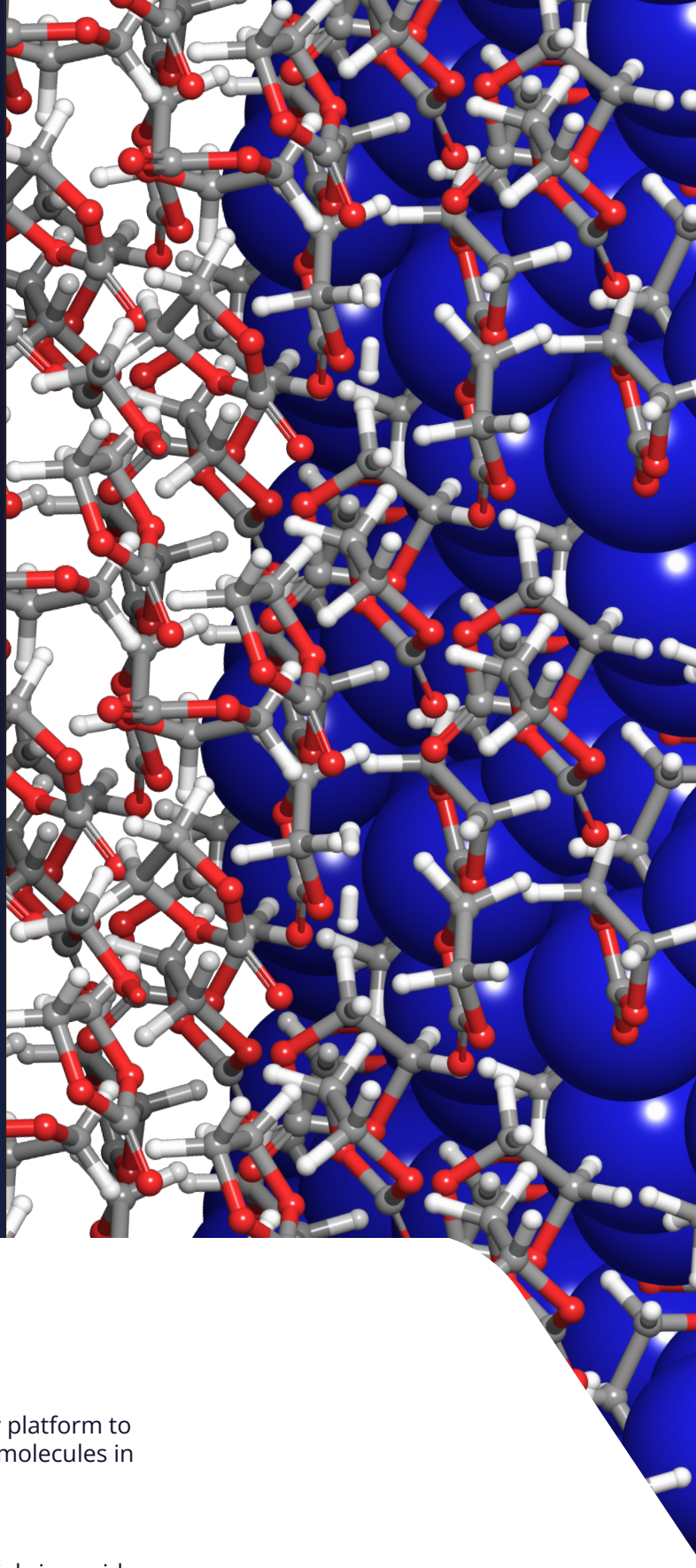
- Capacity and ion intercalation potential
- Ion mobility and kinetics
- Structural and chemical stability

Electrolyte Properties

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



Find the solutions you're looking for:

Drug Discovery

Leverage an industry-leading, integrated digital chemistry platform to explore vast chemical space efficiently and design better molecules in fewer design cycles.

Materials Science

Accelerate the discovery and optimization of novel materials in a wide range of industries and applications with a digital chemistry platform for molecular design and collaboration.

Enterprise Informatics with LiveDesign

Breaks down traditional silo walls to unleash the power of real-time collaborative design and project management.

Schrödinger

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