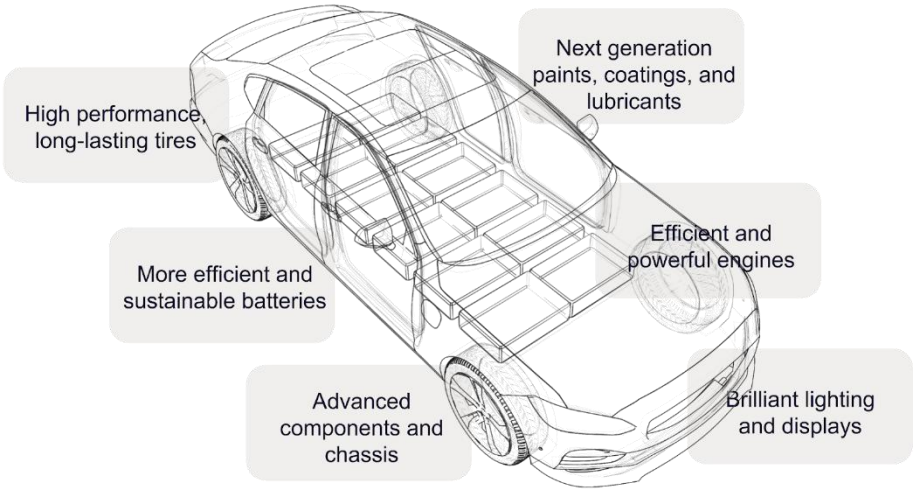
Abstracts

Mathew D. Halls

Senior Vice President
Materials Science
Schrödinger

Advancing Materials Science with Schrödinger: Latest Innovations, Future Roadmap, and Key Applications Impacting the Automotive Industry

The development of advanced materials is crucial for driving technological progress. Schrödinger's digital chemistry platform accelerates this process through atomic-scale modeling, enabling informed selection, discovery, and optimization of materials and processes. Recent advancements in physics-based simulations and machine learning enhance the accuracy, efficiency, and accessibility of Schrödinger software. In recent years, Schrödinger's key areas of development have led to powerful capabilities that impact multiple different materials applications that are critical to the development of future automobiles; examples include polymers for improved tires, battery materials for next generation EVs, optimized formulations for fuels and lubricants, and new display materials for infotainment and lighting.



Garvit Agarwal

Scientific Lead for
Energy Storage
Schrodinger

Harnessing Molecular Simulation and Machine Learning for Rapid Advancements in Battery Materials for Automotive Applications

The rapid advancements in rechargeable Li-ion battery (LIB) technology over the last decade has revolutionized several key industries such as automotive and consumer electronics. However, new battery chemistries are needed to meet the rapidly growing demand and to improve the power density, safety, reliability, and lifetime of LIBs. Molecular modeling has become an integral part of the design cycle of new battery chemistries. Accurate atomic scale modeling enables rapid evaluation and screening of large chemical and material design space thereby, helping industries reduce the time required to bring the new technology to the market.

The presentation will showcase recent technological advancements within Schrödinger's digital chemistry platform, specifically tailored for the design of battery materials. I will discuss examples to illustrate the implementation of automated solutions for the accurate prediction of critical properties in electrode and electrolyte materials, including electrochemical and thermal stability, open circuit voltage, ion diffusivity, and conductivity. Furthermore, the presentation will detail the application of Schrödinger's SEI simulator module, designed to model the nucleation and growth of solid electrolyte interphase (SEI) layers and their correlation with electrolyte composition. Lastly, I will address Schrödinger's latest developments in machine learning force fields for the modeling of complex materials such as liquid and polymer electrolytes, as well as inorganic solid-state materials, thereby facilitating the efficient development of innovative materials for future battery technologies for automotive applications.

Andrea Browning

Senior Director – Polymers
and Soft Matter
Schrödinger

Polymer Digital Tools for Next Generation Transportation Materials

Functional materials such as polymer composites have important role in transportation and other industries. Innovation of polymers and polymer formulations for use in functional materials, requires the balancing of multiple properties. The computational solutions available in the Schrödinger Materials Science Suite have been used in this application space to better understand the relationship between chemical functionality and performance through computational screening of target properties. With the latest releases in 2025, new property workflows are available to extend the design considerations for new materials; such as thin plane shear simulation for solution viscosity. The optimization of complex polymer mixtures is further enhanced with the inclusion of MARTINI automatic particle identification and parameterization in the Coarse Grained Force Field Builder, allowing for the creation of suggested particles for use in the automatic parameterization workflow. This presentation will describe these new solution workflows and show how they are enabling improved design for polymers and complex formulations.

Pavel A. Dub

Product Manager
Catalysis and Reactivity
Schrödinger

Schrödinger Reactivity and Catalysis Tools for Automotive-Related and Functional Materials Simulation

In this presentation, we will showcase our automated workflows for simulating reactivity and catalysis. We will illustrate their capabilities with tailored examples focused on automobile-related and functional materials.

井本 文裕

シニア サイエンティスト

全固体リチウムイオン電池における負極―電解質の界面構造およびLi拡散について

リチウムイオン電池（Lithium Ion Battery: LIB）は1990年代以降、電子機器・車載用バッテリーなどに幅広く利用されています。近年の動向としては、従来の液系電解質には安全性や低エネルギー密度などの欠点があるため、不燃性固体電解質とLi負極を利用した全固体電池が注目されています。ところが全固体電池には、（1）Li負極からの電子移動による固体電解質の還元劣化、（2）Li負極からのLiデンドライト成長といった問題点が知られています。そこで、固体電解質の還元劣化とLiデンドライト成長を防ぐために、Li負極上にBNなどの保護膜（人工SEI）を形成することが試みられており、界面状態の制御が重要です。

本講演では、固体電解質について、負極－保護膜界面および保護膜－電解質界面の安定構造・電子状態、Liが界面を拡散する障壁を理論的に解析した事例をご紹介いたします。特に保護膜候補としてZnO、BN、LiClに注目し、エネルギー的に安定なLi1.3Al0.3Ti1.7(PO4)3 (LATP) 電解質(012)面とLi負極(001)面の間に保護膜を作る構造を計算対象としました。いずれの保護膜についても、(a) Li(001)面－保護膜界面、(b) 保護膜－LATP(012)界面の構造は未解明であるため、界面の安定構造・電子状態・Li拡散障壁を理論的に解析しました。

計算モデルに用いる界面構造は、(a) Li(001)－保護膜および(b) 保護膜－LATP(012)界面を、格子ひずみが10 %以内になるように面間の回転角を変化させることで網羅的に作成しました。これらの界面構造に対し、弊社開発の機械学習力場によりハイスループットな安定構造探索を行いました。Li移動障壁の計算では、Quantum ESPRESSO（QE）の一機能であるNudged Elastic Band法（NEB法）を利用いたしました。Materials Science Suite（MSS）に含まれるQEのNEB法では、弊社にて実装を改良したスキームによる並列化効率の高い計算が可能です。