

NEWS RELEASE

Schrödinger Research Published in Nature Reveals New Insights into Lithium-Ion Battery Chemistry

10/14/2026

New study uncovers multi-lithium ion clustering in common battery electrolytes, paving the way for improved battery performance and design

NEW YORK--(BUSINESS WIRE)-- Schrödinger, Inc. (Nasdaq: SDGR) today announced the publication of new research in Nature that reveals critical insights into the atomic-scale structure of lithium-ion battery (LIB) electrolytes. In a joint study with researchers from Columbia University and the New York Structural Biology Center, the team discovered new insights that challenge long-held assumptions of the fundamental chemistry of lithium-ion batteries, including multi-lithium ion complexes that may play an important role in electrolyte behavior and battery function. These new mechanistic insights into electrolyte behavior have the potential to transform battery development from empirical trial-and-error toward predictive design to high-throughput, rational, computationally-driven design for higher-capacity, faster-charging, and longer-lasting batteries.

The research, which leveraged Schrödinger's physics-powered computational platform, addresses a long-standing bottleneck in energy storage design. LIB electrolytes are crucial for battery performance, influencing properties such as conductivity, viscosity, salt dissociation, and electrochemical stability. LIB electrolytes also drive the formation of the solid electrolyte interphase, which is the critical protective film on the battery anode that dictates battery lifespan and safety. However, a detailed atomic-level understanding of how electrolyte structure impacts these properties had remained limited. Utilizing Schrödinger's advanced machine learning force field technology, the team simulated LIB electrolytes at unprecedented accuracy and scale. These simulations showed that lithium ions frequently form clusters coordinated by ethylene carbonate solvent molecules without the presence of anions, a fundamental structural phenomenon previously unrecognized.

"Simulating complex battery systems has historically forced scientists to choose between quantum precision and

large-scale simulation. Our machine learning force field technology eliminates that trade-off,” stated Mat Halls, senior vice president, materials science, of Schrödinger. “Predicting these multi-lithium complexes and validating them experimentally demonstrates that our platform can detect previously inaccessible chemical phenomena to accelerate materials discovery.”

“Using Schrödinger’s proprietary, advanced machine learning force fields, we discovered lithium ions in batteries actually group together into clusters in the absence of anions, and that these clusters are what drive the creation of the protective film on the battery’s surface,” stated Richard Friesner, co-founder and member of the Board of Directors at Schrödinger, and William P. Schweitzer Professor of Chemistry at Columbia University. “Predicting this unexpected chemistry computationally and confirming it experimentally demonstrates that Schrödinger’s physics-powered platform can accurately model the hidden atomic details of batteries. Furthermore, these results suggest that many, if not most, complex chemical systems are now amenable to predictive physics-based simulation using machine learning force fields to atomic resolution.”

Key Findings:

- **Multi-Lithium Ion Clustering:** In standard battery electrolytes, up to 40% of lithium ions group together into multi-ion clusters, with clustering becoming even more prevalent at higher salt concentrations. This finding upends the long-held assumption that lithium ions remain predominantly isolated in solution.
- **Accurate Experimental Validation:** The machine learning force field simulations demonstrate strong agreement with a wide range of condensed-phase experimental data, including NMR spectra, electrolyte density, viscosity, ionic conductivity, and diffusion coefficients, confirming the physical reality of the predicted multi-lithium clusters.
- **Electrochemical Implications:** Quantum chemical calculations indicate that these multi-lithium clusters have uniquely facile reduction potentials, suggesting they are key intermediates in the formation of the solid electrolyte interphase, which is critical for battery longevity and safety.
- **Foundation for Rational Electrolyte Design:** The insights gained provide a fundamental understanding that can guide the rational design of next-generation electrolytes with enhanced performance, stability, and charge rates.

This research is ongoing and is supported by funding from Gates Ventures.

About Schrödinger

Schrödinger is transforming molecular discovery with its computational platform, which enables the discovery of novel, highly optimized molecules for drug development and materials design. Schrödinger’s software platform is built on more than 30 years of R&D investment and is licensed by biotechnology, pharmaceutical and industrial companies, and academic institutions around the world. Schrödinger also leverages the platform to advance a

portfolio of collaborative and proprietary programs. To learn more, visit www.schrodinger.com, follow us on **LinkedIn**.

Cautionary Note Regarding Forward-Looking Statements

This press release contains forward-looking statements within the meaning of The Private Securities Litigation Reform Act of 1995 including, but not limited to those statements regarding the potential advantages of Schrödinger's computational platform, including the capabilities and potential advantages of its machine learning force field technology, and the potential for computational, physics-based simulation to enable predictive design of batteries and accelerate materials discovery. Statements including words such as "aim," "anticipate," "believe," "contemplate," "continue," "could," "estimate," "expect," "goal," "intend," "may," "might," "plan," "potential," "predict," "project," "should," "target," "will," "would" and statements in the future tense are forward-looking statements. These forward-looking statements reflect Schrödinger's current views about its plans, intentions, expectations, strategies and prospects, which are based on the information currently available to the company and on assumptions the company has made. Actual results may differ materially from those described in these forward-looking statements and are subject to a variety of assumptions, uncertainties, risks and important factors that are beyond Schrödinger's control, including the uncertainties inherent in scientific research, its ability to further develop its computational platform, its reliance on third-party providers of cloud-based infrastructures to host its software solutions, and the ability to retain and hire key personnel on its business and other risks detailed under the caption "Risk Factors" and elsewhere in the company's Securities and Exchange Commission filings and reports, including its Quarterly Report on Form 10-Q for the quarter ended June 30, 2026, filed with the Securities and Exchange Commission on August 5, 2026, as well as future filings and reports by the company. Any forward-looking statements contained in this press release speak only as of the date hereof. Except as required by law, Schrödinger undertakes no duty or obligation to update any forward-looking statements contained in this press release as a result of new information, future events, changes in expectations or otherwise.

Jaren Madden (Investors and Media)

Schrödinger, Inc.

jaren.madden@schrodinger.com

617-286-6264

Matthew Luchini (Investors)

Schrödinger, Inc.

matthew.luchini@schrodinger.com

917-719-0636

Theresa Masnik (Media)

SHIFT Communications

schrodingerpr@shiftcomm.com

212-229-1037

Source: Schrödinger