Optimizing network topology for safer, high-performance batteries

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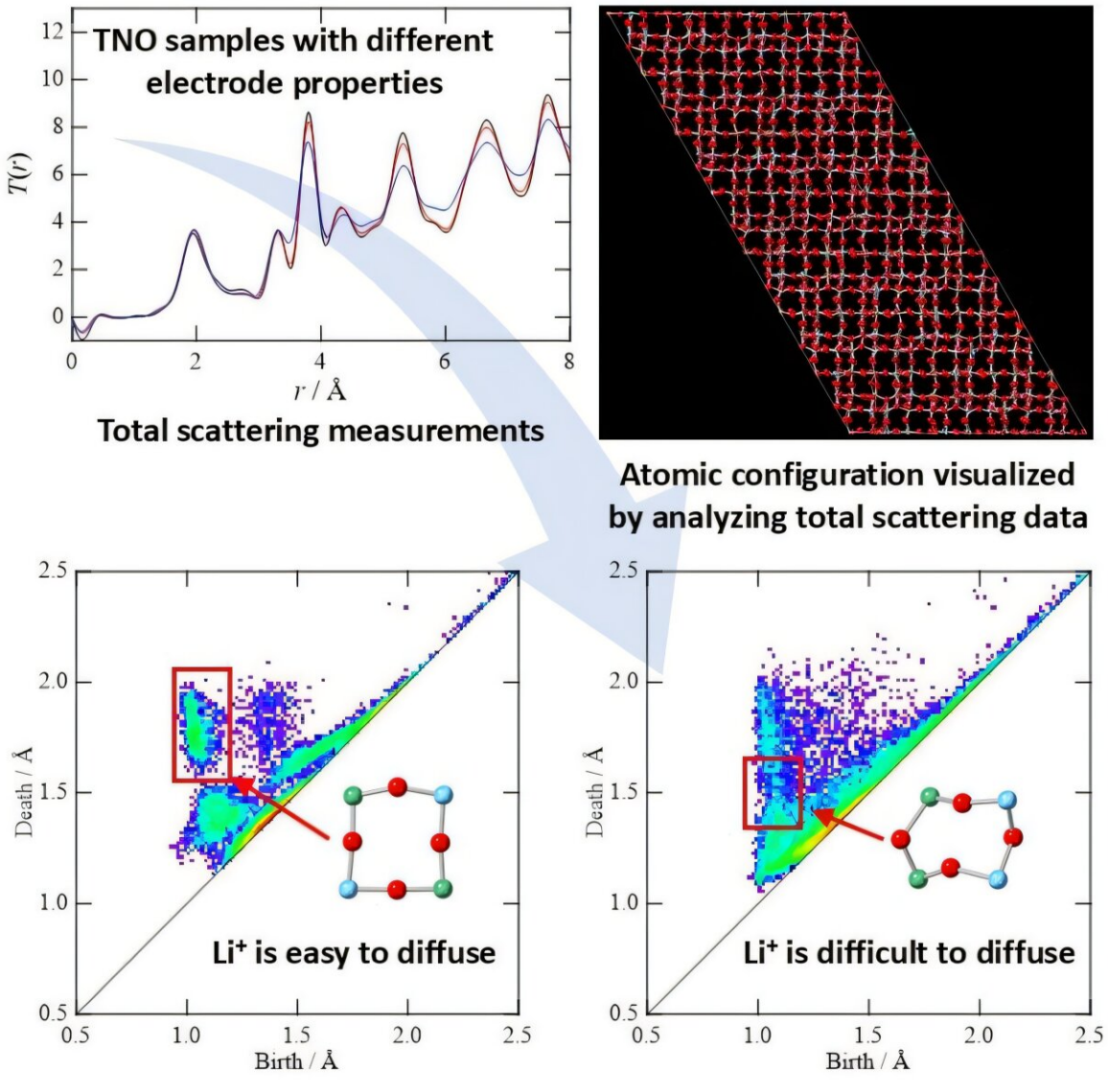

Researchers from Tokyo University of Science developed a three-dimensional atomic structure from scattering data of different TNO samples to examine the factors that affect the negative-electrode properties. The analysis revealed that network disorder significantly affects negative electrode performance and that the topology can be controlled by optimizing the preparation process. Credit: Dr. Naoto Kitamura / Tokyo University of Science, Japan

With rising greenhouse gas emissions, the urgency of addressing global warming and climate change has intensified, prompting a global shift towards renewable energy. The development of rechargeable batteries is essential for this effort.

Lithium-ion batteries (LIBs) are one of the most widely used rechargeable batteries today, being used in cars, smartphones, and even for power storage. However, one major issue with LIBs is the risk of ignition.

Commercial LIBs have a carbon-negative electrode with a low working potential. Since carbon operates near lithium metal deposition potential, there is a risk of internal short circuits, especially when the battery is quickly charged.

Alternative materials for LIB-negative electrodes have been thoroughly studied in recent years, with transition metal oxides. Oxide-based materials operate at a slightly higher potential than lithium, reducing the risk of short circuits. Additionally, they have excellent thermal stability, further reducing fire risk.

Notably, oxide-based negative electrodes behave as insulators in the fully discharged state, insulating the battery in the event of an accident. Despite these advantages, existing oxide-based electrodes, such as

$Li_4Ti_5O_{12}$, have a significantly smaller capacity compared to carbon electrodes, which has prompted research into perovskite-related materials.

Among these materials, Wadsley–Roth phase oxides, like the $TiNb_2O_7$ (TNO), have received considerable attention. However, the atomic structure of TNO remains unknown, essential for understanding and optimizing its negative electrode properties.

To address this gap, a research team from Japan, led by Associate Professor Naoto Kitamura, from the Department of Pure and Applied Chemistry at Tokyo University of Science (TUS), including Mr. Hikari Matsubara, Prof. Chiaki Ishibashi, and others, investigated the atomic structure and the effect of network structure on the electrode properties of TNO.

Their study was published online in the journal *NPG Asia Materials* on December 10, 2024.

"The network structure of TNO forms lithium-ion conduction pathways and has a significant influence on the properties of negative electrodes. However, elucidating such network structures by conventional crystal structure analysis techniques is difficult," explains Prof. Kitamura.

"In this study, we performed reverse Monte Carlo (RMC) modeling using quantum beam data and topological analysis based on persistent homology to explain the factors that affect the negative-electrode properties."

They prepared three TNO samples with distinct charge-discharge properties: a pristine version, a ball-milled sample to reduce the particle size, and a heat-treated sample. Then, they collected total scattering data of the samples from quantum beam measurements and used RMC

modeling to generate a three-dimensional (3D) atomic structure of the materials using the data.

These generated atomic structures reproduced the total scattering data and the Bragg profile data of the real samples, indicating their validity. Further, they conducted topological analysis, based on persistent homology, on the generated 3D structures and thoroughly examined the relationship between the topology of atomic configuration and negative electrode properties in detail.

Their analysis revealed that reducing the particle size by ball milling and subsequent heat treatment, which relaxed the distortion in the network structure, was best for improving charging and discharging capacities.

This suggests that network disorder significantly affects negative electrode performance. Moreover, it shows that the topology can be controlled for the best charging/discharging capacities by optimizing the preparation process.

"For the first time, we could prove that the combination of intermediate-range structure and topology analyses is a promising way of developing a guideline for improving electrode properties," notes Prof. Kitamura.

"TNO can be used in lithium-ion batteries for cars and can contribute to the green growth strategy for achieving carbon neutrality," he adds.

These research insights are instrumental in developing next-generation LIBs with improved safety and capacity, paving the way towards a sustainable, renewable energy-powered future.

More information: Naoto Kitamura et al, Relationship between network topology and negative electrode properties in Wadsley–Roth phase TiNb2O7, *NPG Asia Materials* (2024). DOI:

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