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Optimized crystalline structure in niobium oxide anodes increases lithium-ion battery performance **FREE**

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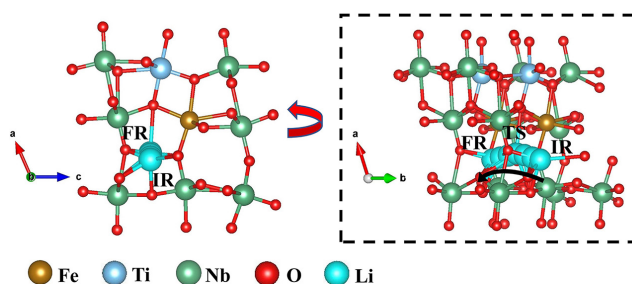
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One-step solution combustion method used for introducing extra cations to enhance the cation-disorder effect.



With accelerating growth in electric vehicles and grid-scale energy storage systems, advances in lithium-ion (Li-ion), the dominant battery technology, continues to be a critical focus. Carbon coating and nanostructure development in anodes are typically used to enhance electrochemical performance, but the methods are complicated and tend to decrease packing density.

To address this challenge, Lv et al. optimized the crystalline structure of niobium oxide, a promising anode material, by enhancing the cation-disorder effect (CDE) in the lattice cell units. They achieved a nearly 72% retention rate after 10,000 cycles. Without optimization, niobium oxide cycle life is typically lower than 5,000.

CDE, the mixing of cations induced by element distribution in the cell unit, contributes to Li-ion diffusion capability and electronic conductivity in the complex Wadsley-Roth crystal structures of niobium oxide.

To regulate CDE, the researchers developed an iron-titanium-niobium-oxide (FTNO) compound using a one-step solution combustion method that added more types of cations within the sublattices. They synthesized the FTNO ($\text{Fe}_{0.67}\text{Ti}_{0.67}\text{Nb}_{1.0}\text{O}_{29}$) solution into a powder, which was mixed with black carbon and coated on copper foil, to build the anode. The anode was paired with a lithium-iron-polonium cathode in a full battery cell.

They found the coexistence of iron and titanium cations (Fe^{3+} and Ti^{4+}) in the crystallographic shear structure enhanced CDE. The optimized lattice structure exhibited short-range order in an irregular quasirectangle-like morphology that contributed significantly to lower charge transfer resistance and a fast Li-ion diffusion rate.

“The overall charge balance between the various cations and oxygen anions is achieved in the enhanced cation-disorder effect, contributing to a remarkably stable structure for prominent electrochemical performance,” author Cheng Chao Li said.

Source: “Cation mixing in wadsley-roth phase anode of lithium-ion battery improves cycling stability and fast li+ Storage,” by Zeheng Lv, He Zhu, Weiwei Meng, Licheng Wei, Yang, Yufei Zhang, Minghui Ye, and Cheng Chao Li, Applied Physics Review (2021). The article can be accessed at <https://doi.org/10.1063/5.0054030>.

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