Topological Quantum Materials for the Anode and Cathode of Metal-Ion Batteries

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The 2019 Nobel Prize in Chemistry and the 2016 Nobel Prize in Physics were awarded for groundbreaking research on lithium-ion batteries and topological quantum materials, respectively, both of which have significantly advanced their respective fields. An intriguing question arises: how can these two domains be interconnected? A key motivation for answering this question stems from the US Advanced Battery Consortium’s goal of developing fast-charging electric vehicle batteries capable of reaching 80% capacity within 15 minutes. This ambitious target necessitates novel electrode materials with both high ionic and electrical conductivity. In response, topological quantum materials—distinguished by electronic band structures that differ fundamentally from conventional metals and insulators—have emerged as promising candidates due to their intrinsically high and topologically protected electrical conductivity.Since our pioneering study in 2017 [PNAS 114, 651 (2017)], this area has garnered substantial attention. In this talk, we summarize our research progress, focusing on 3D porous topological semimetal anodes composed of light elements such as boron, carbon, and silicon for Li, Na, and K-ion batteries. On the cathode side, leveraging machine learning techniques—including support vector machines, Gaussian process regression, decision trees, and atomic line graph neural networks—we screened 7,358 topological quantum materials and identified LiMnAs, Na_4CoO_3, and K_2MnS_2 as the most promising cathode candidates for Li, Na, and K-ion batteries. These materials exhibit high reversible capacities, high energy densities, multiple transport channels with low energy barriers, and minimal volume changes during charge-discharge cycles. Our findings not only open a new avenue for designing high-performance electrode materials beyond conventional options but also expand the application landscape of quantum materials, bridging the gap between topological quantum physics and battery technology.

References

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