frontiers | Frontiers in Materials

TYPE Editorial
PUBLISHED 17 February 2025
DOI 10.3389/fmats.2025.1550721

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RECEIVED 23 December 2024
ACCEPTED 05 February 2025
PUBLISHED 17 February 2025

CITATION
Benedek NA, Radovic M, Goodge BH and De la Torre A (2025) Editorial: Symmetry-guided rational design and control of quantum matter with new functionality.
Front. Mater. 12:1550721.
doi: 10.3389/fmats.2025.1550721

Editorial: Symmetry-guided rational design and control of quantum matter with new functionality

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KEYWORDS

quantum materials, symmetry, superconductivity, local structure, magnetism, spintronics application

Editorial on the Research Topic
Symmetry-guided rational design and control of quantum matter with new functionality

Quantum materials provide a vibrant playground to challenge our comprehension of complex emergent phenomena and a vital foundation for disruptive next-generation technologies. Ongoing advances in rational material design, synthesis approaches, ultrafast optical control, and experimental and theoretical characterization tools can be deployed in a continuous dynamic feedback loop to probe the fundamental nature of complex matter and achieve tunable control of their functional properties. This Research Topic showcases recent work in the design and control of quantum materials, including new observations, predictions, and methodologies that further our current understanding of their emerging properties.

In particular, our Research Topic includes four articles on a wide range of Research Topic, from prediction to synthesis to understanding new materials. Abarca Morales introduces a framework designed to analyze and predict materials' structures and symmetries, especially how they evolve under strain. By focusing on the interactions and arrangements of four interconnected octahedra—a common motif in many quantum materials—this model provides insights into the emergence of specific material functionalities and facilitates the rational design of compounds with desired characteristics. Focusing on materials properties, Han et al. reviews the potential of ABO_3 transition metal oxides (TMOs) in spintronic applications. Emphasis is put on their unique electronic structures and quantum states, discussing how the interplay between strong spin-orbit coupling and electronic correlations leads to efficient charge-spin interconversion. It highlights strategies for tuning these properties through epitaxial strain and heterostructure engineering. Nixon et al. presents a new study on superconducting mercurides of strontium, offering valuable insights into superconductivity in mercury-rich compounds and addressing the challenges of synthesizing these materials by studying their structural and superconducting properties. Finally, Romaguera and Medarde focuses on the design principles for stabilizing magnetoelectric (ME) spiral phases at room temperature. Recent experimental observations in Cu/Fe-based layered perovskites demonstrate how chemical disorder and control over specific interatomic distances can stabilize magnetic spiral phases at temperatures as high as 400 K. The review presents strategies for designing materials with ME spirals suitable for practical applications. Altogether, this Research Topic reflects the breadth of knowledge needed to tackle the challenges and opportunities in the design and control of quantum materials.

These articles underscore the transformative power of combining prediction and experiment to push the boundaries of what is possible in quantum science. Other examples not shown in this Research Topic include the dimensionality control in thin films of Ruddlesden-Popper transition metal oxides, which have emerged as a key platform to control their emergent properties (Kim et al., 2017; Pan et al., 2022; Spencer et al., 2024). Topotactic reactions in Kitaev iridates have provided a versatile approach to manipulate and tailor their magnetic and electronic properties towards the elusive Quantum Spin Liquid limit (Bahrami et al., 2022) Additionally, machine learning is rapidly transforming the field of quantum materials by enabling predictive capabilities that were previously unattainable. For example, predictions involving materials such as LiBC highlight the potential to establish novel superconducting phases (Tomassetti et al., 2024a; Tomassetti et al., 2024b). By leveraging large datasets and advanced algorithms, machine learning provides a powerful tool to guide experiments and theory, bridging the gap between materials discovery and functional applications.

We are deeply grateful to the authors, reviewers, and editors who have made this Research Topic possible. Their collective efforts have resulted in a diverse and impactful Research Topic of works highlighting the importance of symmetry-guided approaches in advancing quantum materials. We hope this Research Topic inspires new ideas and directions in the discovery, engineering, and functionalization of quantum materials for next-generation computing, sensing, and energy technologies.

Author contributions

NB: Writing–original draft, Writing–review and editing. MR: Writing–original draft, Writing–review and editing. BG: Writing–original draft, Writing–review and editing. AD: Writing–original draft, Writing–review and editing.

Funding

The author(s) declare that no financial support was received for the research, authorship, and/or publication of this article.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Generative AI statement

The author(s) declare that no Generative AI was used in the creation of this manuscript.

Publisher's note

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