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Speaker

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Talk Title

Precision Materials Design for Reticular Spintronics

Abstract

Reticular spintronics seeks to exploit the structural and chemical programmability of reticular materials to design and control unconventional spin functionalities. Metal-organic frameworks (MOFs), with their modular metal nodes, organic linkers, coordination environments, and diverse network topologies, provide an attractive platform for establishing systematic structure-spin-function relationships. In this work, I will present a theoretical framework for the precision design of spin functionalities in reticular materials, with a particular focus on the emerging altermagnetism and fully compensated ferrimagnetism. The design framework is developed from three complementary perspectives: symmetry, chemistry, and orbital degrees of freedom. From a symmetry perspective, spin-space symmetry provides a foundation for establishing the relationship between crystal structure and spin degrees of freedom, enabling the identification and design of unconventional magnetic states. From a chemical perspective, the choice of metal nodes, organic linkers, and coordination environments provides chemical control over magnetic interactions and magnetic ground states. From an orbital perspective, orbital engineering and orbital hybridization offer additional control over the electronic structure and spin-dependent properties, enabling the targeted tuning of magnetic states and spin splitting. Overall, these design principles provide a systematic framework for the rational design of magnetic reticular materials and their spin functionalities.

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Short biography

Dr. Yixuan Che is currently a Humboldt Research Fellow (Global Minds Initiative Germany) at the Chair of Theoretical Chemistry, Technische Universität Dresden. He received his B.Sc. in Materials Chemistry from University of Science and Technology of China (USTC) in 2022 and Ph.D. in Materials Physics and Chemistry at the Hefei National Research Center for Physical Sciences at the Microscale, USTC, in 2026, under the supervision of Prof. Xiaojun Wu. During his doctoral studies, he was selected as a member of the National Advanced Talent Cultivation Center for Chemistry (2024–2026). His research focuses on the theoretical design and physical modeling of low-dimensional reticular materials, with particular interests in chemically programmable magnetic states, altermagnetism, topological phenomena, and emergent spintronic functionalities.