Frontier Interdisciplinary Strategy

Research Report on Frontier Interdisciplinary Research and Judgment of Molecular Spin Science and Technology

Frontier Interdisciplinary Research and Judgment of Molecular Spin Science and Technology Research Team

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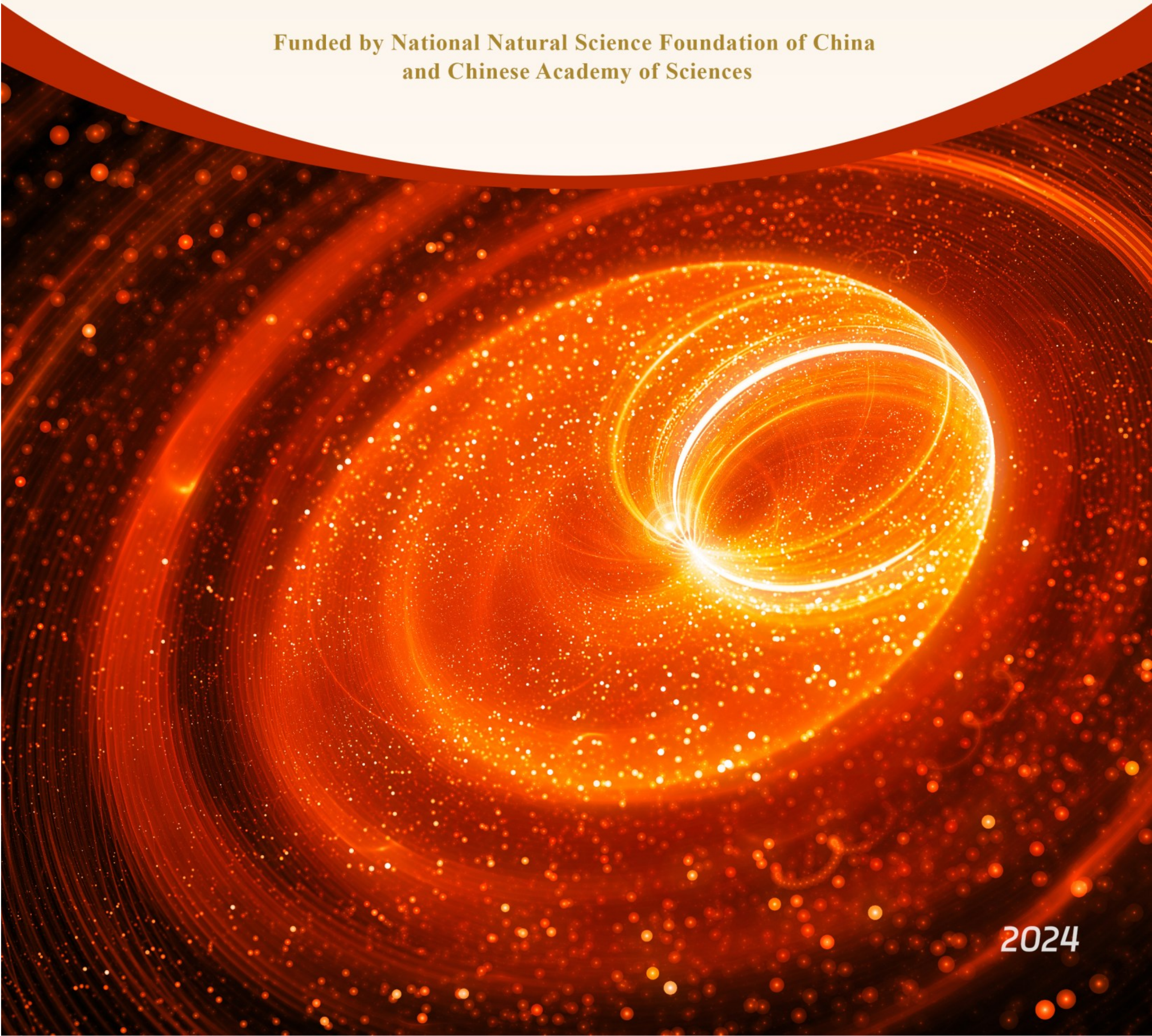

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Abstract

Molecular spin science and technology has emerged as an interdisciplinary field focusing on electron spins in molecules and related applications in physics, chemistry, biology, materials science, and information science. It will play a crucial role in technological innovations. The chemistry of spins is deeply related to the essence of chemical bonds, chemical catalysis, enzyme catalysis, optical and electromagnetic properties, quantum computation and quantum precision measurements. The related research is intersectional, cutting-edge and has a wide range of application prospects. This report introduces the strategic value of science and technology related to molecular spins, analyses the current status and trend in relative research domestically and internationally, extracts key scientific questions and technological difficulties in the field, and provides suggestions on the development of the field in China.

Content

Chapter 1 THE STRATEGIC VALUE OF MOLECULAR SPIN SCIENCE AND TECHNOLOGY

Spin is an intrinsic property of electrons and other fundamental particles on the quantum level. Since the birth of quantum mechanics approximately 100 years ago, the technological advancement of the world paralleled with our growing knowledge of the spins.

Research of traditional chemistry focuses on molecules' geometric structures, steric effects, charge distribution and their effects on the physical and chemical properties of matter, as well as reaction rates and product and chirality selectivity. Electron spins have provided a new degree of freedom which is less studied. Spin effects in chemical reactions can inspire new high-performance catalysts, synthesis methods and reaction paths.

Spins have been a major focus in physical research, but studied mostly in a range of limited systems. As carriers of electron spins, molecular materials have advantages of mass production and atomic uniformity, and therefore can help in our understanding of magnetism from the microscopic level and the development of magnetic materials. The quantum behaviors of molecules can be modulated through chemical synthesis. Upcoming quantum and spintronic information technologies greatly rely on spin materials including molecule-based multiferroic materials, bipolar magnetic semiconductors and molecular qubits.

The fusion of physics into chemistry and biology is still insufficient. Interdisciplinary activities may allow researchers to solve long-standing problems such as the spin-involving mechanisms in chemical and biological processes. The study of molecular spin involves collaborative efforts to understand the fundamental behaviors of electrons within molecules. More important is that the research outcomes in this field have the applicational potential which may lead to industrial innovation and upgrading. This field has always been a highly competitive area internationally and is a key area in the scientific and technological deployments of developed countries.

Chapter 2 KEY SCIENTIFIC QUESTIONS IN MOLECULAR SPIN SCIENCE AND TECHNOLOGY

In this Interdisciplinary Frontier Assessment Project focused on molecular spin science and technology, 8 seminars were held, themed “molecular spin-electric interactions”, “molecular spin-optic interactions”, “intrinsic correlation between molecular spins and chirality”, “spin relaxation”, “new phases based on molecular spins”, “molecular spins in biomedicine”, “spin effects in chemical reactions” and “photoelectric radicals”. More than 120 experts in chemistry, physics, biology, medicine, and materials science attended, extracted the following key scientific questions in multiple research and application scenarios, and call for interdisciplinary efforts to address them.

(i) How to achieve efficient spin polarization in molecules?

Spin polarization refers to biased spin microstate populations. Thermal population are often insufficient, while light-pumping, using spin-selective transitions, offers a promising alternative. Developing relative approaches in molecular systems needs deep theoretical understanding and systematic experimental exploration.

(ii) What is the essential relation between molecular spins and molecular chirality?

From a physics perspective, spin breaks time reversal symmetry, while chirality breaks spatial inversion symmetry. Understanding the intrinsic link between spin, charge, and chirality could unify these properties in molecular systems, potentially addressing major questions such as the origin of chirality in living organisms. Current challenges include a deeper understanding of how chiral molecules respond to external angular momentum.

(iii) How to achieve magnetoelectric coupling in molecular

systems?

Achieving magnetoelectric coupling in molecular solids can unify electric and magnetic properties, enabling faster, more localized, and energy-efficient spin manipulation. This is crucial for advancing spintronics and quantum computing, where electric control of magnetic states is essential for high-density storage and scalable quantum bit operations.

(iv)How to readout spins on the single-molecule level?

Traditional studies of molecular spins mainly aim at collective ensemble averages. While informative, relative methods are limited in detecting the quantum nature of individual molecular spins. Techniques like single-molecule readout using electrical and optical methods face challenges due to weak signals and short coherence times, calling for further technological advancements.

Chapter 3 DOMESTIC AND INTERNATIONAL RESEARCH FOUNDATION AND CONDITIONS

Molecular spin science and technology emerges from collective progress in multiple fields including coordination chemistry, free radical chemistry, chemical catalysis, biomedicine, semiconductor physics, quantum information and spintronics. It has grown into a vibrant cutting-edge multi-disciplinary field, including but not limited to the following frontier areas.

(i) Spin effects in chemical reactions, which influence reaction pathways, product types, yields, and rates by altering spin states and microstates, often through spin-orbit coupling and can be modulated by external magnetic fields.

(ii) Spin effects in molecular materials, especially those with novel magnetic and multifunctional properties, including room-temperature molecular ferromagnets, molecular nanomagnets and molecular quantum information materials.

(iii) New phases in molecular spin materials, achieved through precise topological and lattice spin state engineering, in which one can realize frustrated structures like honeycomb and Kagome, enabling the study of possible quantum spin liquids and various other cutting-edge problems in condensed-matter physics.

(iv) Molecular spins in diagnostic and therapeutic agents, including MRI contrast agents developed based on molecular spins to enhance MRI signals while having better bio-safety and specificity, heat-induced thrombolytic drugs, and medicine that can intervene in disease signaling via spin states.

(v) Theoretical computation of molecular spins, which is essential for understanding and exploiting molecular spins. Theoretical and computational tools should adapt to the development of experiment technologies to meet the challenges brought by new findings.

Chapter 4 DEVELOPMENT STRATEGIES AND POLICY RECOMMENDATIONS

Molecular spin science and technology interconnects with multiple disciplines. Considering its major features which are interdisciplinarity, innovativeness and applicability, we propose strategies and policy recommendations of:

(i) breaking down disciplinary barriers by diverse course developing and research team fostering,

(ii) emphasizing solid foundations and broad perspectives in higher education,

(iii) differentiating between free exploration and goal-oriented research to establish evaluation systems that align with the nature of either type,

(iv) prioritize the development of indigenous scientific instruments and strengthen collaboration with enterprises, and

(v) establishing major national science and technology projects focused on molecular spin science and technology to promote breakthroughs, convert research into productive innovations, and cultivate young talents.

Developing molecular spin science and technology promotes deep integration of chemistry, physics, biology, and information science, and is an important path towards interdisciplinary exploration, paradigm transformation, and original innovation.