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Theoretical and Computational Aspects of Magnetic Organic Molecules

Sambhu N Datta, Carl O Trindle, Francesc Illas

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Organic materials with extraordinary magnetic properties promise a wide range of light, flexible, and inexpensive alternatives to familiar metal-based magnets. Individual organic molecules with high magnetic moments will be the foundation for design and fabrication of these materials.

This book provides a systematic understanding of the structure and properties of organic magnetic molecules. After a summary of the phenomenon of magnetism at the molecular level, it presents a survey of the challenges to theoretical description and evaluation of the magnetic character of open-shell molecules, and an overview of recently developed methods and their successes and shortfalls. Several fields of application, including very strong organic molecular magnets and photo-magnetic switches, are surveyed. Finally, discussions on metal-based materials and simultaneously semiconducting and ferromagnetic extended systems and solids point the way toward future advances.

The reader will find a comprehensive discourse on current understanding of magnetic molecules, a thorough survey of computational methods of characterizing known and imagined molecules, simple rules for design of larger magnetic systems, and a guide to opportunities for progress toward organic magnets.

Readership: Theoretical and computational chemists, synthetic organic chemists, condensed matter physicists, material scientists and engineers. Material scientists and engineers looking to enter a new field of application. Graduate students, post doctoral fellows, and faculty members in chemistry, physics, materials science and a variety of engineering specialties.

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