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Strategies towards High-Temperature Lanthanide-Based Single-Molecule Magnets

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Lanthanide-based single-molecule magnets are leading materials for achieving magnetization blocking at the level of one molecule. In this presentation, the physical requirements for efficient magnetization blocking in single-ion complexes will be examined and the design principles for achieving very high magnetization blocking barriers in lanthanide-based compounds will be identified[1]. It will be shown that the key condition is the preponderant covalent binding of the Ln ion to one of the ligand atoms, tremendously enhancing the axial crystal field. I will also make an overview of practical schemes for the implementation of this principle[2]. These are (1) the effective lowering of the coordination number via displacement of the Ln ion to one of the atoms in the coordination polyhedron, (2) the design of two-coordinated complexes, and (3) the stabilization of diatomic compounds in cages and on surfaces. The last proposal is appealing in connection to spintronics applications, especially via the exploration of robust and highly anisotropic [LnX] units displaying multilevel blocking barriers of thousands of Kelvin and prospects for room-temperature magnetization blocking. Finally, the effect of exchange and magnetic dipolar interactions of lanthanide with other magnetic centers on the magnetization blocking will be shortly discussed[3]. The conditions allowing to achieve highly opaque blocking barrier due to these interactions will be revealed. [1] L. F. Chibotaru, "Theoretical understanding of anisotropy in molecular nanomagnets," Struct. Bond. 164, 185-229 (2015). [2] L. Ungur and L. F. Chibotaru, Inorg. Chem. 55, 10043 (2016). [3] L. F. Chibotaru, "Exchange interaction in lanthanides", J. Phys.: Cond. Matter, in preparation.