

3rd International Conference on Quantum Materials and Technologies

## Powerful Single-Molecule Magnets Containing Radicals and Bismuth



Date and Time:
From 26 April to
3 May 2025, exact
day&time will be
announced later.

Lecture Room: TBD

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## Distinguished Professor Selvan Demir

Selvan Demir is an Assistant Professor of Chemistry (tenuretrack) at Michigan State University. She developed a highly productive research program in which her group synthesizes peerless molecules with the aim to overcome current limits in spin science. The bigger picture is to construct new compounds with rare earth (RE) metals, heavy p-block elements (e.g. bismuth), and organic radicals to generate coveted room-temperature single-molecule magnets (SMMs) which hold promise to revolutionize applications in highdensity information storage, quantum computing, and spinbased electronics. Her unique approach delicately controls oxidation states, spin states and magnetic exchange coupling of the RE metals and ligands through clever molecular design employing organic and inorganic chemistry. She published 52 research papers, where 18 were featured on the front covers of journals. Furthermore, she delivered 126 invited seminars to chemistry and physics communities in 25 countries. She received numerous awards such as the Klaus Liebrecht-Award, the NSF CAREER award, the ACS WCC 2025 Rising Star award, and the Friedrich Wilhelm Bessel Research Award by the Alexander von Humboldt Foundation.

She received her PhD in Chemistry from the University of Cologne in 2010 researching on scandium chemistry with Prof. Gerd Meyer and Prof. William J. Evans at the University of California, Irvine. Subsequently, she conducted postdoctoral studies with Prof. Jeffrey R. Long at the University of California, Berkeley, and Dr. David K. Shuh at Lawrence Berkeley National Laboratory. She was a Junior Professor of Inorganic Chemistry at the University of Göttingen before moving to Michigan State University in January 2019.

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10th International Conference on Superconductivity and Magnetism

## **Abstract**

Lanthanides are qualified candidates for the construction of singlemolecule magnets (SMMs) owing to their large magnetic moments and high magnetic anisotropy that stem from strong spin-orbit coupling of the 4f orbitals. By using lanthanide ions such as Tb(III) and Dy(III) which possess intrinsically large orbital angular momentum, substantially higher spin-reversal barriers and blocking temperatures can be attained. One effective methodology to boost blocking temperatures of multinuclear compounds is to generate strong magnetic exchange between lanthanide centers using radical bridging ligands. In the event of large magnetic exchange coupling, undesirable relaxation pathways such as quantum tunneling of the magnetization can be suppressed. Here, the first isolation of the bisbenzimidazole radical anion (Bbim3-•)and its use in radical-bridged SMMs will be discussed, Fig. 1.1,2 Furthermore, the isolation of the first fluoflavine radicals will be presented, which are promising for the design of radical-bridged SMMs.3 A second approach to strong coupling employs heavy p-block elements since their diffuse valence orbitals facilitate better penetration of the core electron density of the lanthanide ions relative to diamagnetic ligands comprising lighter p-block elements. Here, we will present the first lanthanide bismuth cluster SMMs containing a [Ln2Bi6] heterometallocubane core, Fig. 1.4 We will also show that the Bi23-• radical anion can be tamed with rare earth ions to give the first SMMs featuring bismuth radicals, Fig. 1.5 By contrast, the methodology to enhance SMM properties in mononuclear lanthanide complexes is to match the ligand field symmetry with the anisotropic electron density distribution of the maximal MJ state, which we also probed by isolating new compounds that will be discussed.

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