

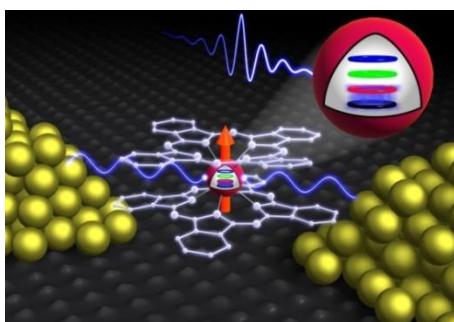
# Quantum Computing with Molecules

## Mario Ruben

INT, IQMT, Karlsruhe Institute of Technology (KIT), Karlsruhe/D  
ISIS, CESQ, University of Strasbourg, Strasbourg/F

[mario.ruben@kit.edu](mailto:mario.ruben@kit.edu)

Metal complexes will be proposed to act as active quantum units for Quantum Computing (QC). We report on the implementation of metal complexes into nanometre-sized (single-)molecular spintronic devices by a combination of bottom-up self-assembly and top-down lithography techniques. The controlled generation of magnetic molecular nanostructures on conducting surfaces/electrodes will be shown and persistence of their magnetic properties under confinement in Supramolecular Quantum Devices (SMQD) will be proven. The quantum behaviour (e.g.. superposition, entanglement) of the metal complexes will be addressed at the single molecule level<sup>1-13</sup> to finally implement a quantum algorithm on a TbPc<sub>2</sub> Qudit performing quantum computing operations.<sup>10</sup>



**Figure 1** Artistic representation of a Molecular Spin Transistor based on a TbPc<sub>2</sub> complex acting as a molecular Spin Qudit.<sup>8</sup>

### References:

- [1] S. Kyatskaya et. al. *J. Am. Chem. Soc.* **2009**, *131*, 15143-15151.
- [2] M. Urdampilleta et al. *Nature Mater.* **2011**, *10*, 502-506.
- [3] J. Schwöbel et. al. *Nature Comms.* **2012**, *3*, 953-956.
- [4] R. Vincent et al. *Nature* **2012**, *488*, 357-360.
- [5] M. Ganzhorn et al. *Nature Nano.* **2013**, *8*, 165–169.
- [6] M. Ruben et. al. *Nature Nano.* **2013**, *8*, 377–389.
- [7] S. Wagner et. al. *Nature Nano.* **2013**, *8*, 575–579.
- [8] S. Thiele, et al. *Science* **2014**, *344*, 1135-1138.
- [9] M. Ganzhorn, et. al. *Nature Comms* **2016**, *7*, 11443.
- [10] C. Godfrin et al. *PRL* **2017**, *119*, 187702 (perspective article by A. Morello *Nature Nano* **2018**, *13*, 9-10).
- [11] H. Biard et. al. *Nature Comms* **2021**, *12*, 4443.
- [12] S. Kuppusamy et. al. *Nature Comms* **2021**, *12*, 2152.
- [13] D. Serrano et al. *Nature* **2022**, *603*, 241.

### Recent Reviews:

"Molecular Spin Quddits for Quantum Algorithms."

E. Moreno-Pineda, C. Godfrin, F. Balestro, W. Wernsdorfer, M. Ruben. *Chem. Soc. Rev.* **2018**, *47*, 501.

„Synthetic Engineering of the Hilbert Space of Molecular Quddits: Isotopologue Chemistry.“

W. Wernsdorfer, M. Ruben. *Adv. Mat.* **2019**, *31*, 1806687.