Scientific Area	Developing quantum hardware
Topic title	Synthetic Engineering of the Hilbert Space of Lanthanide Complexes for Quantum Gates and Algorithms
Main host institution	KIT www.kit.edu
Supervisor/institution	Mario Ruben (KIT) www.ruben-group.de
Co-Supervisor/institution	J. Klinovaia, Uni Basel : https://www.quantumtheory.unibas.ch/people/klinovaja/
Mentor[1]/institution	S Klyatskaya, KIT: https://www.int.kit.edu/staff_svetlana.klyatskaya.php
Secondment institution	Uni Basel, D. Loss : https://www.quantumtheory.unibas.ch/people/loss/

Topic description

In lanthanide (*Ln*) compounds, the localized *4f*-electrons interact both, with the itinerant *spd* electrons as well as with each other, leading to a rich variety of unusual properties of interest for quantum information sciences [1,2]. It was previously shown, that the long coherence time of the nuclear states residing in the lanthanide molecular magnets make these compounds suitable Qudit candidates (e.g. with d = 4, see ref 3). We have shown that the Grover´s quantum algorithm can be realised in a single molecule employing a Hadamard gate to create a superposition of the nuclear states of the Tb(III) (m_I = ±1/2 and ±3/2) [4]. By a Grover evolution, which amplifies the amplitude of the searched state, previously labelled spin states, via its phase or its energy, can be used as quantum register. The Grover´s algorithm yields a quadratic speed up, compared to classical algorithms, by operating on systems with a high superposition of states.
The task of the project consists now in the synthetic engineering of the Hilbert Space of lanthanide complexes using Isotopological Chemistry [5]: the achievement of the Grover's algorithm in a single molecule was possible due to the four different nuclear states embedded in the $[TbPc_2]^0$ molecule and the distinct separation between the levels. Logically, more complex and demanding algorithms could be executed with a larger number of available (for computation) states larger than 4 (d > 4). In this context, chemistry offers all necessary tools to achieve such goal, such as by engineering the dimension, topology, and symmetry of the Qudit by the selection of the appropriate lanthanide centre tailoring the correct nuclear spin multiplicity.

The experiments will be carried out in synthetic chemistry laboratories to ensure a clean and reproducible experimental environment. The candidate will participate in an ambitious multi-partner project within Gen-Q including strong support from experimental and theoretical physics. In our research team, the PhD students receive all the necessary information and support to seek a job at the end of PhD thesis. Our PhD students, without exception, find a job in academics or industry.

References

[1] Mentor: The primary role of the mentors will be to identify and facilitate specific training objectives, advise on any problems faced by the ESR, including career matters with an external perspective and provide mediation in the case of disputes.

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[1] S. Thiele et. al. *Science* **344**, 1135 (2014); [2] R. Vincent, et. al. *Nature* **488**, 357 (2012) [3] C. Godfrin et al. *PRL*, **119**, 187702 (2017) (perspective article in *Nature Nano* **13**, 9-10 (2018). [3] E. Moreno-Pineda, C. Godfrin, F. Balestro, W. Wernsdorfer, M. Ruben, *Chem. Soc. Rev.* **47**, 501 (2018) [5] W. Wernsdorfer, M. Ruben, *Adv. Mat.* **31**, 1806687 (2019).

Recommended applicant's profile

We are looking for a highly motivated candidate with a master degree in chemistry or chemical-physics. The candidate for this PhD project must have strong background in molecular chemistry or physics. Core competence in synthetic chemistry in required, additional experience in ultrahigh vacuum, scanning tunneling microscopy, or material science is welcome. A strong will to collaborate with partners doing the theoretical physics and proficiency in English are required. Interested candidates are invited to send a CV, a motivation letter, grades and ranking along with two supporting letters. The candidate will be selected in agreement with the application procedure of the Gen-Q PhD school, after an audition and a job interview.

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