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# #ICMolTalks


## *Alessandro Lunghi*

***Trinity College Dublin***


27th May at 12:00h

Assembly Hall

***Computational Design of Magnetic Molecules: from ab initio simulations to high-throughput molecular discovery***

## Abstract


Magnetic molecules have been proposed as key elements of novel technologies, ranging from spintronics, quantum sensing and high-density information storage, but their integration with complex environments at room temperature stands out as a main road block.

Among the many challenges in this area, one of the most crucial ones is the stabilization of the coherence of magnetic molecules' spin at high temperature. Spin-lattice interaction is the main limitation to the spin lifetime in insulating materials, but its theoretical formulation is mostly based on a phenomenological approach and a quantitative understanding of its microscopic origin is often lacking. In addition to this uncertainty on the nature of spin-lattice interactions, the goal of actually translating new design principles into chemical strategies poses some serious challenges to the field.

In this seminar I will discuss how computational modelling can play a pivotal role in the design and discovery of new magnetic molecules with long spin coherence time by taking care of most of – if not all - the essential steps in this process: i) provide a deep understanding of the physics driving spin decoherence, and ii) discover new molecules with ideal properties.

In the first part of the seminar I will detail the recent successes in usign ab initio methods to describe spin relaxation in realistic molecular systems of arbitrary complexity, e.g. going from simple S=1/2 to highly correlated Lanthanide ions [1-3]. In the second part of the seminar I will show how ab initio methods can come together with machine learning and high-performance computing to enable high-throughput exploration of magnetic molecules' chemical space, de facto accelerating the discovery of molecules with long spin lifetime [4].



References:
[1] M. Briganti, et al. The Journal of the American Chemical Society, 143, 13633–13645 (2021)
[2] A. Lunghi. Science Advances, 8, eabn7880 (2022)
[3] S. Mondal, A. Lunghi, The Journal of the American Chemical Society, 144, 22965-22975 (2022)
[4] A. Lunghi, Nature Reviews Chemistry 6 (11), 761-781 (2022)


## Biography

Alessandro holds a Ph.D. in computational inorganic chemistry, received in 2016 from the University of Florence. His Ph.D. dissertation focused on the computational and theoretical investigation of molecular magnets and their interaction with typical solid-state environments. In 2016 he joined the School of Physics at Trinity College Dublin as a research fellow and started working on designing machine-learning methods for accelerating molecular dynamics simulations of solid-state materials. In 2020 he was awarded a European Research Council Starting Grant and in 2021 he was appointed as Assistant Professor in Physics at Trinity College Dublin, where is now leading a growing research group. Alessandro's interests lie at the boundary between open quantum systems theory, ab initio modelling, materials design and machine learning and his group is leaveraging this highly multidisciplinary set of techniques to discover novel magnetic molecules with long coherence times for quantum technologies.