
PhD studentship position at Trinity College Dublin in Machine-Learning and First-Principles Modelling of Molecular Qubits and Molecular Nano-Magnets.

Background

A fully funded 4-year PhD studentship is available at the School of Physics, Trinity College Dublin, Ireland (www.tcd.ie/Physics). The position is sponsored by the host institution and the European Research Council through the Starting Grant AI-DEMON: Artificial Intelligence Design of Molecular Nano-Magnets and Molecular Qubits.

The aim of this project is to push the boundaries of the state-of-the-art in the computational modelling and design of magnetic molecules. The interaction between spins and phonons is one of the main limits to the development of spin quantum technologies and in this project we will use first-principles and machine-learning methods to unravel the details of spin-phonon coupling and develop new magnetic molecules with long spin coherence and lifetime[1-5]. The project will be developed by the group of Prof. Lunghi at the School of Physics, Trinity College Dublin, and in close collaboration with leading experimental groups in the field.

What we offer

The appointee will take part to a 4-year PhD program in Physics hosted by Trinity College Dublin and will be supported by a tax-free stipend of EUR 18,500. College fees will be met by the funding source. Together with other members of the Quantum Materials Dynamics research group, the new student will have the opportunity to be a key player in a cutting edge research project and fully develop their potential in a supportive and friendly environment. The appointee will receive a top-class training in computational physics/chemistry and machine learning and will develop a very innovative research profile in computational condensed-matter physics.

What we are looking for

The ideal candidate is a talented and motivated student that successfully completed their undergraduate studies and is now looking for a place to further develop their own scientific and research skills. The candidate will be required to contribute to the research group by actively participating to scientific discussions and creating a supportive work environment. Among the main technical tasks, they will be expected to contribute to the overall efforts of the research group by developing a computational framework able to design molecular compounds with long spin lifetime. This will involve the design of novel software that brings together machine-learning and ab initio methods, liase with experimental collaborators, and publish scientific papers in the main international journals. Interests and experience in scientific dissemination and outreach will also be positively considered.

Essential Selection Criteria

- A BSc or a MSc in Physics, Chemistry, or another related scientific discipline, with at least a 2.1 honors grade from an Irish university or equivalent.
- Good spoken and written English;
- Understanding of the basic principles of quantum mechanics and/or electronic structure theory and/or microscopic theory of magnetism;
- Experience with linux environments and basic knowledge of programming, e.g. Fortran, Python, Julia and C/C++;

Application Procedure

All the correspondence regarding this position, including informal inquiry and formal application, should be addressed to Prof. Alessandro Lunghi (lunghia@tcd.ie).

Applications must include:

- 1) A cover letter detailing how you meet the selection criteria for the post;
- 2) A complete academic CV;
- 3) A sample of scientific output, e.g. a chapter of the thesis;
- 4) The e-mail contacts of at least two referees who have agreed to provide a reference letter;

Review of the applications will start on the 1st of March 2023 at the latest and the position will remain open until a suitable candidate is identified. A first round of interviews is expected to be held no later than the 1st of April 2023 and will be held remotely. The selected candidate will be invited to enroll in the PhD programme to start no later than September the 1st 2023. The enrollment process may involve an English assessment and further reference checks (www.tcd.ie/courses/postgraduate/how-to-apply/requirements).

Equal Opportunities Policy

Trinity is an equal opportunities employer and is committed to employment policies, procedures and practices which do not discriminate on grounds such as gender, civil status, family status, age, disability, race, religious belief, sexual orientation or membership of the travelling community. On that basis we encourage and welcome talented people from all backgrounds to join our staff community.

References

- [1] Science Advances, 5, eaaw2210 (2019)
- [2] The Journal of the American Chemical Society, 143, 13633-13645 (2021)
- [3] Science Advances, 8, eabn7880, (2022)
- [4] The Journal of the American Chemical Society, 144, 22965-22975 (2022)
- [5] Nature Reviews Chemistry, 6, 761-781 (2022)