Postdoctoral fellowship at Trinity College Dublin in Machine-Learning Design of Molecular Qubits and Nano-Magnets.

Background

A 2-year postdoc position is available at the School of Physics, Trinity College Dublin, Ireland (www.tcd.ie/Physics). The position is sponsored by 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 methods to unravel the details of spin-phonon coupling and develop new magnetic molecules with long spin coherence and lifetime[1-4]. The group is also strongly pursuing the development of machine-learning schemes for the exploration of structure-magnetic properties maps[5-7], and the appointed postdoctoral researcher will develop generative machine-learning models to steer the design of new compounds with long coherence and spin relaxation times. The project will be developed by the group of Prof. Lunghi at the School of Physics, Trinity College Dublin, (www.tcd.ie/Physics/research/groups/quantum-materials-dynamics/) and in close collaboration with leading experimental groups in the field.

What we offer

The appointee will join the group of Prof. Lunghi at the School of Physics of Trinity College Dublin and together with other members, they 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. The appointment will initially be made for 1 year and with a gross annual salary in the order of EUR 42,000. Upon successful performance during this initial period, a one-year extension of the contract will be offered to the candidate. A starting date as late as November the 1st 2023 is possible.

What we are looking for

The ideal candidate is a strongly motivated researcher that is looking for a place to 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, co-supervise undergraduate and postgraduate students, and publish scientific papers in the relevant international journals. Interests and experience in scientific dissemination and outreach will also be positevily considered.

Selection Criteria

Essential:

• A Ph.D. (or a recently submitted thesis awaiting evaluation) in Physics, Chemistry, or another related scientific discipline;

• Understanding of the basic principles of quantum mechanics and/or electronic structure theory;

• Experience in at least one of these programming languages: Python, Julia, FORTRAN, C/C++;

• Good spoken and written English and the ability to work both independently and in a team;

• Strong motivation to advance the project by pro-actively developing personal ideas.

Highly Desirable:

• Experience in the development of machine-learning models and use of software such as PyTorch or TensorFlow;

• Experience with the use of High Performance Computing platform and parallel programming/computing.

• Experience in the use of quantum chemistry and periodic DFT electronic structure codes, such as CP2K, quantum espresso and ORCA;

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 including a full list of scientific output;
3) 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 April 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 mid-May / early-June and will be held remotely.

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] Science Advances, 5, eaaw2210, (2019)
[6] Physical Review B 105 (16), 165131 (2022)
[7] Nature Reviews Chemistry, 6, 761-781 (2022)