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

Project Background
A 3-year research fellow position is available from January 2021 at the School of Physics, Trinity College Dublin (Ireland). 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 five-year project is to push the boundaries of the state-of-the-art in the computational modelling of magnetic molecules and design new compounds with optimal properties. The interaction between spins and phonons is one of the main limits to the development of spin quantum technologies. 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[1-4]. The project will be developed by the group of Dr. Lunghi at the School of Physics, Trinity College Dublin, and in close collaboration with leading experimental groups in the field, such as the groups of Prof. Sessoli (www.lamm.unifi.it) and Prof. Torre (www.lens.unifi.it) at the University of Florence. The project will also avail of collaborations with the CRANN (www.tcd.ie/crann/) and AMBER (www.ambercentre.ie/) research centres, in particular with the groups of Prof. Sanvito and Prof. Wolfgang Schmitt.

Research Fellow Duties
• The main focus of the project will be on one or more of the following topics, depending on the appointee previous experience:
  • Development of machine-learning models to predict molecular properties at the first-principles level of accuracy [1,2];
  • Application of spin relaxation theory to magnetic molecules with in-house developed codes [3,4];
  • Development and implementation of new algorithms to predict spin relaxation;
• Help with the supervision of under/post-graduate students and project development;
• Write manuscript for publication in the main peer-reviewed international journal;
• Disseminate results by participating to the main conferences in the field.

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 and/or microscopic theory of magnetism;
• Experience in the use of unix/linux environments and at least one programming language. Preferred programming languages are Fortran(standard 2003 or later), Python, Julia and C/C++;
• Respect for all colleagues, collaborators and students, regardless of their personal status and background;
• 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.
Desirable:
• Experience in the use of quantum chemistry and periodic DFT electronic structure codes, such as CP2K, quantum espresso and ORCA;
• Experience in the training of machine-learning models and use of software such as PyTorch or TensorFlow;
• Experience in the theory and modelling of quantum systems and their dynamics;
• Experience with the use of High Performance Computing platform and parallel programming/computing.

Application Procedure
All the correspondence regarding this position, including informal inquiry and formal application, should be addressed to Dr. 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 November 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 December and will be held remotely.

Selection Procedure
The appointment will initially be made for 1 year and with a maximum gross annual salary of EUR 42,200 (IUA Salary Scale Level 2.4). Upon successful performance during this initial period, a two-year extension of the contract will be offered to the candidate. A starting date as early as 1st January 2021 may be possible.

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