Trinity College Dublin
The University of Dublin

CRANN

One PhD position open in quantum transport in magnetic devices

One PhD position is available for a March 2021 entry in the School of Physics and the CRANN Institute (www.crann.tcd.ie) at Trinity College Dublin (Ireland). Sponsored by Science Foundation of Ireland (SFI) this is part of the "materials for ICT" platform of the AMBER research center (ambercentre.ie). The project will be hosted by the *Computational Spintronics Group* (www.spincomp.com), headed by Prof. Sanvito, and will be strongly connected to the experimental activity at CRANN and AMBER. The project will include methodological algorithm development and materials science.

Quantum transport for magnetic devices

The PhD position is part of the "materials for ICT" platform of the AMBER research center and aims at developing computational methods for quantum transport in nanodevices. In particular our focus will be that of combining quantum transport and magnetization dynamics to explore current induced dynamics in nanoscale junctions, incorporating antiferromagnets and/or highly compensated ferrimagnets [see for instance M.O. Ellis, M. Stamenova and S. Sanvito. *Multi-scale modelling of current-induced switching in magnetic tunnel junctions*. Phys. Rev. B **96**, 224410 (2017)]. The methods used combine the non-equilibrium Green's function method for electron/spin, as implemented in the Dublin-based *Smeagol* code [A.R. Rocha, V.M. Garcia Suarez, S.W. Bailey, C.J. Lambert, J. Ferrer and S. Sanvito. *Spin and Molecular Electronics in Atomically-Generated Orbital Landscapes*. Phys. Rev. B **73**, 085414 (2006); www.tcd.ie/Physics/Smeagol/], with atomistic micromagnetic simulations.
The project will be tightly related to the experimental activity of the groups of Prof. Coey and Prof. Stamenov in the School of Physics and AMBER, and strong collaboration between theory and experiments is envisage. The student will be supervised by Prof. Sanvito and Dr. Stamenova.

Essential/Desirable Criteria

Strong overall motivation and a keen interest in theory and computation, as well as in interdisciplinary work between physics and materials science. Previous experience in UNIX/Linux environment and with programming in either Fortran and/or C/C++. Ability to work independently and also function as an active and efficient team player. Good writing skills. Previous knowledge of density functional theory and/or electronic structure methods will be considered as an advantage. Previous experience with micromagnetic methods is also welcome.

How to apply?

Applications must include a cover letter detailing how you meet the selection criteria for the post, together with a CV and the name and contact details of at least two referees (e-mail address). Informal inquiring and applications should be sent to:

Prof. S. Sanvito (Trinity College Dublin, sanvitos@tcd.ie)

Information about the research group can be found at: http://www.spincomp.com. The position will be open until filled.

Trinity College Dublin
The University of Dublin

CRANN

Trinity College Dublin

Trinity College Dublin is Ireland's university on the world stage. Recognized for its transformative research and education conducted at the frontiers of disciplines, Trinity is ranked 61st in the world by the QS World University Rankings 2013. Spread across 47 acres in Dublin's city centre, Trinity has a 17,000-strong student body, 3,000 staff and over 100,000 alumni around the world. Of the student body, 16% come from outside Ireland and, of those, 40% are from outside the European Union, making Trinity's campus cosmopolitan and bustling, with a focus on diversity. Trinity has developed significant strength in a broad range of research areas, including the 21 broadly based multi-disciplinary thematic research areas.
See www.tcd.ie/research/themes.

CRANN

CRANN, the Centre for Research on Adaptive Nanostructures and Nanodevices (www.tcd.ie/crann), is Ireland's first purpose-built research institute. CRANN is focused on delivering world-class research and innovation through extensive proactive collaborations with industry and is committed to attracting and training graduate students to the highest international standards. CRANN works at the frontiers of nanoscience developing new knowledge of nanoscale materials, with a particular focus on new device and sensor technologies for ICT, the biotechnology and medical technology sectors and a growing interest in energy related research. The institute employs a team of over 300 researchers from 45 different countries, led by 30 principal investigators, each of whom is an internationally recognized expert in their field of research, which include physics, chemistry, medicine, biochemistry and immunology, engineering and pharmacy.
Since its inception in 2003, CRANN has greatly assisted in radically transforming Ireland's international reputation for research. A Thomson Reuters report in late 2010 placed Ireland 8th globally for materials science research based on citations per publication for the decade 2000-2010. CRANN researchers were responsible for > 70% of the outputs leading to this national ranking. In Nanotechnology, Ireland's global ranking is sixth in terms of both the quality of its publications and the volume output per capita.

AMBER

AMBER (Advanced Materials and BioEngineering Research - ambercentre.ie) is a world-leading SFI Research Centre funded by Science Foundation Ireland, hosted by Trinity College Dublin which provides a partnership between leading researchers in materials science and industry to develop new materials and devices for a range of sectors, particularly the ICT, medical devices and industrial technology sectors. Working in collaboration with CRANN (Trinity's Centre for Research on Adaptive Nanostructures and Nanodevices), the Trinity Centre for Bioengineering and with University College Cork and the Royal College of Surgeons in Ireland.

Trinity College Dublin
The University of Dublin

CRANN

2 postdoc positions open in Computational Materials Design at Trinity College Dublin

Two postdoc positions are available from as early as February 2021 in the School of Physics and the CRANN Institute (www.crann.tcd.ie) at Trinity College Dublin (Ireland). Both projects will be hosted by the *Computational Spintronics Group* (www.spincomp.com), headed by Prof. Sanvito, and are strongly connected to the experimental activity at CRANN and the AMBER center (ambercentre.ie). The projects will include methodological algorithm development and computational materials science. The successful candidates will also be asked to take some responsibility in PhD-student supervision and project management.

The initial deadline for submission is **January the 15th, 2021**.

Position 1: Design of metal-organic frameworks for gas capture and conversion

The position will be part of a large project aiming at the computational design of novel metal-organic frameworks (MOFs) for CO_2 capture and conversion. We will use machine-learning methods trained over large experimental and theoretical datasets to explore a vast chemical and structural space. These will provide a first pool of materials prototypes, whose electronic and structural properties will be calculated with advanced electronic structure theory (density functional theory) operated in a automatized high-throughput mode. Then, for the most promising materials, we will construct state-of-the-art machine learning force fields and with these explore their finite-temperature behaviour. Feedback between the different levels of theory will be essential, so that the results of the force fields and of density functional theory will enable the improvement of the machine-learning models. In particular we will implement force fields capable to capture chemical reactions, and efficient schemes to map complex potential energy surfaces.

The project will maintain a close collaboration with experimental groups at Trinity (Profs. Schmitt and Nicolosi) and at the University of Limerick (Prof. Zaworotko), who will attempt the synthesis of the most promising MOFs identified by the theory. The project is, in fact, integrated in the "Energy" research platform of the AMBER center at Trinity College. The appointment will be made for 1 year in the first instance, with possibility for extension, up to 3 years in total. This is desirable and dependent on the appointee's performance. A start date as soon as February 2021 may be possible. The successful candidate will be supervised by Prof. Sanvito and by Prof. Lunghi, both in the School of Physics at Trinity College Dublin.

Position 2: Theory of emergent magnetism

The interface between two materials can be used to engineer new properties that neither component could exhibit separately (emergence). Furthermore, it is a materials strategy that can be used for the tuning of capabilities found in of one of them (enhancement), or for sharing their functionalities (proximity). Here, we will use molecular interfaces to generate novel magnets, to control the spin properties of thin films, and to add functionalities. From a fundamental point of view, the origin of these experimentally observed effects is not yet fully explained due to the complexity of the interfaces, the materials involved, and their intricate quantum-electronic properties. Our aims are:

i. To develop a new theoretical framework to study magneto-molecular coupling and interfaces, accounting for the many physical factors at play in the coupling between metals and molecules.

ii. To improve the properties of commonly-used magnetic thin films via nanocarbon overlayers.

iii. To create the opportunity for switchable magnetism by turning on/off the interfacial spin ordering using electric fields.

Trinity College Dublin
The University of Dublin

CRANN

The Researcher will play a central role within a newly-launching international research collaboration "Emergent Magnetism and Spin Interactions in Metallo-Molecular Interfaces", which brings together Trinity's Computational Spintronics (Prof. S. Sanvito) and Condensed Matter Theory (Prof. D. O'Regan) and Groups, the U.K. STFC Scientific Computing Department (Dr G. Teobaldi), and exciting experimental work at the University of Leeds, U.K. (Dr O. Cespedes and Prof. B. J. Hickey). The appointment will be made for 1 year in the first instance, with possibility for extension, up to 3 years in total, which is desirable and dependent on the appointee's performance. A start date as soon as February 2021 ma y be possible. The successful candidate will be supervised by Prof. Sanvito and by SFI-Royal Society University Research Fellow, Dr. Droghetti.

Essential/Desirable Criteria

Strong overall motivation and a keen interest in theory and computation, as well as in interdisciplinary work between physics and materials science. Previous experience in UNIX/Linux environment and with programming. Ability to work independently and also function as an active and efficient team player. Good writing skills. Previous knowledge of density functional theory and/or other electronic structure methods will be essential. Experience with MOFs and with force fields methods (position 1), and with magnetism and magnetic materials (position 2), and/or with machine-learning methods (both positions) will be considered as an advantage.

How to apply?

Applications must include a cover letter detailing how you meet the selection criteria for the post, together with a CV and the name and contact details of at least two referees (e-mail address). Informal inquiring and applications should be sent to:

Prof. S. Sanvito (Trinity College Dublin, sanvitos@tcd.ie)

Information about the research group can be found at: http://www.spincomp.com. The position will be open until filled.

Trinity College Dublin, the University of Dublin is an equal opportunities employer and is committed to the 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.

Trinity College Dublin
The University of Dublin

CRANN

Trinity College Dublin

Trinity College Dublin is Ireland's university on the world stage. Recognized for its transformative research and education conducted at the frontiers of disciplines, Trinity is ranked 61st in the world by the QS World University Rankings 2013. Spread across 47 acres in Dublin's city centre, Trinity has a 17,000-strong student body, 3,000 staff and over 100,000 alumni around the world. Of the student body, 16% come from outside Ireland and, of those, 40% are from outside the European Union, making Trinity's campus cosmopolitan and bustling, with a focus on diversity. Trinity has developed significant strength in a broad range of research areas, including the 21 broadly based multi-disciplinary thematic research areas.
See www.tcd.ie/research/themes.

CRANN

CRANN, the Centre for Research on Adaptive Nanostructures and Nanodevices (www.tcd.ie/crann), is Ireland's first purpose-built research institute. CRANN is focused on delivering world-class research and innovation through extensive proactive collaborations with industry and is committed to attracting and training graduate students to the highest international standards. CRANN works at the frontiers of nanoscience developing new knowledge of nanoscale materials, with a particular focus on new device and sensor technologies for ICT, the biotechnology and medical technology sectors and a growing interest in energy related research. The institute employs a team of over 300 researchers from 45 different countries, led by 30 principal investigators, each of whom is an internationally recognized expert in their field of research, which include physics, chemistry, medicine, biochemistry and immunology, engineering and pharmacy.
Since its inception in 2003, CRANN has greatly assisted in radically transforming Ireland's international reputation for research. A Thomson Reuters report in late 2010 placed Ireland 8th globally for materials science research based on citations per publication for the decade 2000-2010. CRANN researchers were responsible for > 70% of the outputs leading to this national ranking. In Nanotechnology, Ireland's global ranking is sixth in terms of both the quality of its publications and the volume output per capita.

AMBER

AMBER (Advanced Materials and BioEngineering Research - ambercentre.ie) is a world-leading SFI Research Centre funded by Science Foundation Ireland, hosted by Trinity College Dublin which provides a partnership between leading researchers in materials science and industry to develop new materials and devices for a range of sectors, particularly the ICT, medical devices and industrial technology sectors. Working in collaboration with CRANN (Trinity's Centre for Research on Adaptive Nanostructures and Nanodevices), the Trinity Centre for Bioengineering and with University College Cork and the Royal College of Surgeons in Ireland.