Trinity College Dublin
The University of Dublin

CRANN

PhD positions open in machine-learning methods for materials science

Several PhD positions are available from September 2019 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) and the Irish Research Council (IRC) these are part of a large effort for developing and implementing machine-learning methods for materials modeling. The projects will be hosted by the *Computational Spintronics Group* (www.spincomp.com), headed by Prof. Sanvito, and are strongly connected with the experimental activity at CRANN and the AMBER research center (ambercentre.ie). All projects will include methodological algorithm development and materials science.

1) *Machine-learning design of novel magnets (several positions available)*

The PhD positions will be part of a large project aiming at the computational design of novel magnets for a range of applications (electric motors, data storage, sensing, antennas, etc.). 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 magnetic properties will be calculated with advanced electronic structure theory (density functional theory) operated in a automatized high-thoroughput 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. The project will maintain a close collaboration with experimental groups at Trinity, who will attempt the synthesis of the most promising magnets identified by the theory. Part of the research will be conducted in collaboration with Prof. Curtarolo's Materials Lab at Duke University. Position will be available in:

1a) Construction of machine-learning models based on theory and experimental data for magnetism.
1b) High-throughput magnetic materials design with advanced electronic structure theory.
1c) Development of machine-learning force fields for spin dynamics.

2) *Multiscale modelling of spin-transport devices*

The aim of the project is to model the interplay between spin-polarised currents and the magnetic structure of materials. This interplay can be exploited in a multitude of memory, logic and combined memory-logic devices, where the currents can be used for both reading and writing the information. The theoretical tool of choice will be quantum transport theory implemented with state-of-the-art electronic structures, computed at the level of density functional theory. Furthermore, the dynamics of the magnetization induced by the currents will be computed with atomistic spin-dynamics tools, namely by solving the micromagnetic problem at the atomic level. The theoretical work will be integrated in a larger effort, which includes the growth and characterization of devices, in the groups of Prof. Coey and Prof. Stamenov, also at Trinity College.

3) *Machine learning methods for ultra-high fidelity microscopy*

Ultramicroscopy defines a range of techniques to resolve the structure of materials at the atomic level. These can include electron-, ion- and light-optical methods. The CRANN Institute operates a state-of-the-art microscopy facility, in particular in the area of transmission electron microscopy (TEM), and it is seeking to continuously improving the methods and accuracy with which we characterize materials. The aim of this project is to develop new methods, rooted in machine learning, image processing and artificial intelligence, for enhancing and expanding today's measurement capabilities. In particular our goal is to be able to process and display information in real-time (live). This will allow us to then tailor the measurement approach in the optimal way for extracting the desired information. For instance we are aiming to resolve the atomic structure of small nanoparticles, defective 2D materials, metallorganic frameworks and organic matter while using a lower electron-beam radiation dose. The project will be supervised jointly by Prof. Stefano Sanvito and Prof. Lewys Jones, both in the School of Physics and CRANN.

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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. For position 3) previous experience with electron microscopy is 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.

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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.