



Trinity College Dublin
The University of Dublin



CRANN

4-year postdoc position open in machine-learning methods for materials science

A 4-year postdoc position is available from September 2019 in the School of Physics and the CRANN Institute (www.crann.tcd.ie) at Trinity College Dublin (Ireland). Sponsored by the Irish Research Council (IRC) this is part of a large effort for developing and implementing machine-learning methods for materials design. The project will be hosted by the *Computational Spintronics Group* (www.spincomp.com), headed by Prof. Sanvito, and is strongly connected to the experimental activity at CRANN and the AMBER research center (ambercentre.ie). The project will include methodological algorithm development and materials science. The successful candidate will also be asked to take some responsibility in PhD students supervision and project management.

The position 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-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 level 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. The project will maintain a close collaboration with experimental groups at Trinity (Profs. Coey and Stamenov), 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.

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 magnetism and magnetic materials and/or with machine-learning methods 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.



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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.