PI name & contact details:	**Prof. Cormac McGuinness – Cormac.McGuinness@tcd.ie**
School: ***Has project been agreed with head (or nominee) of proposed registration school?***	**School of Physics** ***yes***
Research Centre / group affiliation:	**School of Physics – X-ray Spectroscopy and Surface and Interface Physics groups**
Research group / centre website:	**http://www.tcd.ie/Physics/People/Cormac.McGuinness/Research/ and http://www.tcd.ie/Physics/Surfaces/**
PI website / link to CV:	**http://www.tcd.ie/Physics/people/Cormac.McGuinness/**

Brief summary of PI research / research group / centre activity (2 or 3 lines max):
The measurement of the electronic structure and magnetic behaviour of single crystal, doped and defect-ridden binary and ternary transition metal oxides, nitrides and fluorides; capped ordered nanowires and organic molecular semiconductor interfaces, all by synchrotron radiation based x-ray emission spectroscopy (XES), x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD) at EU synchrotron radiation facilities. These spectroscopies are coupled with both laboratory based x-ray photoemission (XPS), LEED, MOKE, I-V measurements, XRD and STEM as well as computational modelling of the materials within TCD.

Title & brief description of PhD project (suitable for publication on web):

Probing chemical bonding in transition metal oxides and fluorides through symmetry selective x-ray spectroscopies

The nature of the chemical bond is of fundamental interest as it is the interplay between the physical structure and chemical bonding in a material which gives rise to the electronic bandstructure and the properties. Photon-in/photon-out x-ray absorption/emission spectroscopy or resonant inelastic x-ray scattering, is elementally selective and can probe either end of a metal-anion chemical bond in a transition metal fluoride or oxide binary compound, impossible by any other method. This can be exploited in e.g. MnF_2 a rutile transition metal fluoride and prototypical antiferromagnet, as well as other MA_2 systems in which the anion (oxygen or fluorine) is sp^2 hybridised. In these due to the anisotropy of the chemical bonding and crystal structure, there is a combination of polarisation dependence (dichroism) and symmetry- and state-selectivity in the observed RIXS/RXES e.g. at the fluorine K edge. This gives separate probes of the differing occupied σ-like and π-like Metal-Anion-derived molecular orbitals that contribute to the electronic bandstructure in these systems. We seek to measure and model this polarisation dependent RXES at the anion K-edge and especially in metal 2p-3d RIXS, how this varies with d-shell filling across the transition metal period, and connect with models of the electronic bandstructure to derive further insight into chemical bonding in these materials. Thus we will measure the symmetry dependent resonant x-ray emission spectroscopy (RXES) or resonant inelastic x-ray scattering (RIXS) for a variety of structurally similar transition metal fluorides and oxides. Epitaxial thin films or bulk single crystal samples of these materials will either be synthesised or obtained. X-ray absorption spectroscopy (XAS) and x-ray emission spectroscopy (XES) measurements will take place at synchrotron radiation facilities principally within the EU.

Unique selling points of PhD project in TCD:
projects should offer something that's not available in Brazil – specific equipment, multi-disciplinarity, aspects of structured programme, links with industry, placements, links with other research groups etc.

The PIs research group routinely access EU based synchrotron radiation sources such as MAXlab in Sweden for our synchrotron radiation based x-ray spectroscopic measurements. The PI has also been a frequent user of the Advanced Light Source in the Lawrence Berkeley Laboratory in California for many measurements. The facilities within TCD in the X-ray Spectroscopy and Surface and Interface physics groups include UHV growth, LEED, MBE deposition and in-situ XPS and UPS measurements as well as equipment dedicated to in-situ I-V and surface optical measurements. In addition, the CRANN institute has very capable nanoscience and advanced microscopy laboratories which feature state of the art equipment relevant to the preparation and characterisation of nanostructures including STM, AFM, STEM, EELS, FIBs and a He Ion microscope.

The Trinity PhD is a structured PhD and students can access discipline-specific training, as well as generic and transferable skills. All PhD students are eligible to participate in the Innovation Academy which offers a Postgraduate Certificate in Innovation and Entrepreneurship to assist PhD students identify and exploit the value within their research.

Name & contact details for project queries, if different from PI named above:

Please indicate the graduates of which disciplines that should apply:
Physics or Materials Science graduates

Ciência sem Fronteiras / Science Without Borders Priority Area:
Please indicate the specific programme priority area under which the proposed PhD project fits- choose only one (tick box):

Engineering and other technological areas	
Pure and Natural Sciences (e.g. mathematics, physics, chemistry)	
Health and Biomedical Sciences	
Information and Communication Technologies (ICTs)	
Aerospace	
Pharmaceuticals	
Oil, Gas and Coal	
Renewable Energy	
Minerals	
Biotechnology	
Nanotechnology and New Materials	X
Technology of prevention and remediation of natural disasters	
Biodiversity and Bioprospection	
Marine Sciences	
Creative Industry	
New technologies in constructive engineering	