<table>
<thead>
<tr>
<th>PI name &amp; contact details:</th>
<th>Dr. Thomas Archer and Professor Stefano Sanvito</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>School:</strong></td>
<td>School of Physics and Crann</td>
</tr>
<tr>
<td><strong>Has project been agreed with head (or nominee) of proposed registration school?</strong></td>
<td>yes</td>
</tr>
<tr>
<td><strong>Research Centre / group affiliation:</strong></td>
<td>Computational spintronics group</td>
</tr>
<tr>
<td><strong>Research group / centre website:</strong></td>
<td><a href="http://www.spincomp.eu/">http://www.spincomp.eu/</a></td>
</tr>
<tr>
<td><strong>PI website / link to CV:</strong></td>
<td><a href="http://www.tcd.ie/physics/people/tom.archer">http://www.tcd.ie/physics/people/tom.archer</a></td>
</tr>
</tbody>
</table>

**Brief summary of PI research / research group / centre activity (2 or 3 lines max):**
The quantum mechanical equations provide an accurate description of nano-devices, however these equations are too difficult to solve. In the spintronics group we work on simplifying these equations to describe how matter behaves on the nanoscale.

**Title & brief description of PhD project (suitable for publication on web):**
Materials genome: In a similar way to how the human genome was mapped we intend to predict the existence of every possible material, only about 100,000 materials are known to science given the size of the periodic table there must be many more to discover, offering unknown and possibly technologically important properties. In this project we will use computational modelling to analyze trends in these newly predicted materials.

**Unique selling points of PhD project in TCD:** We collaborate internationally with many research groups most notably for this project we have a fruitful collaboration with Professor Stefano Curtarolo from Duke University, who is developing the "AFLOW" code for high-throughput computing. We have over 3000 compute cores available on campus 1000 of which are solely for the use of our research group.
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, computational chemistry and applied mathematics

**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