



## Role profile

<b>Job title</b>	Research Associate / Fellow in Theoretical Design of Spin Defects in Quantum Sensors	<b>Job family and level</b>	Research and Teaching Level 4/4A
<b>School/ Department</b>	School of Chemistry	<b>Location</b>	University Park Campus

### Purpose of role

The purpose of this role is to undertake research developing theoretical models to characterise the optoelectronic properties of point defects in semiconductor materials, such as the nitrogen vacancy centre in diamond, guiding the design of enhanced quantum sensing protocol and the development of novel materials for quantum sensing applications.

The Research Fellow will form part of a multidisciplinary team including members of the nanomaterials group in the School of Chemistry and the optics and photonics group in the Faculty of Engineering, working closely with experimentalists in Nottingham and with international collaborators on the development of quantum sensing technology.

The person appointed will be expected to plan and conduct a programme of research in this area with a high degree of independence, employing both advanced wavefunction and density functional theories, making extensive use of high-performance computing resources. They will be responsible for writing up their work for publication and contributing to the preparation of new funding proposals.

The person appointed will have the opportunity to use their initiative and creativity to identify areas for research, develop research methods and extend their research portfolio.

	<b>Main responsibilities</b> (Primary accountabilities and responsibilities expected to fulfil the role)	<b>% time per year</b>
1	<p><b>To plan and conduct research modelling the optoelectronic characteristics of point defects in semiconductors, including:</b></p> <ul style="list-style-type: none"> <li>▪ Development of theoretical methodology to model the effects of magnetic fields on the optoelectronic properties of defects in semiconductors with quantitative accuracy, combining both wavefunction and density functional theories.</li> <li>▪ Proposing new experimental protocol for quantum sensing using defects in semiconductors derived from theoretical investigation to overcome the limitations of present methodology.</li> </ul> <p>Undertake theory-led design of novel defects in semiconductors with properties favorable for quantum sensing of magnetic materials with atom-level precision.</p>	65%

2	<p><b>Write high quality scientific articles for publication in high-impact international peer-reviewed journals, including:</b></p> <ul style="list-style-type: none"> <li>▪ Theory-led publications reporting the developments carried out by the Research Fellow.</li> </ul> <p>Contributing the theoretical analysis to the research outputs of the wider multidisciplinary collaboration.</p>	10%
3	<p><b>Identify and develop new directions for research to advance quantum sensing with defects in semiconductors, including:</b></p> <ul style="list-style-type: none"> <li>▪ Help to develop new multidisciplinary research concepts, both with colleagues and external collaborators.</li> </ul> <p>Contribute to the preparation of new research proposals for submission to external funding agencies.</p>	10%
4.	<p><b>Deliver presentations to disseminate theoretical developments to both internal and external audiences, including:</b></p> <ul style="list-style-type: none"> <li>▪ Participate in regular team meetings to share knowledge / skills and discuss ideas with colleagues.</li> </ul> <p>Disseminate work by contributing to external meetings and conferences, nationally and internationally, when possible.</p>	5%
5.	<p><b>Provide support and participate in knowledge exchange with colleagues and students where appropriate, including:</b></p> <ul style="list-style-type: none"> <li>▪ Guidance to colleagues and instruction to students on theoretical concepts within the Research Fellow's own area of expertise.</li> </ul> <p>Training to assist colleagues and students in accessing and utilizing computational resources effectively.</p>	5%
6.	<p><b>Develop new relationships with academic collaborators as appropriate, including:</b></p> <ul style="list-style-type: none"> <li>▪ Identifying prospective new collaborative projects with external academic partners.</li> </ul> <p>Contribute proactively to advancing collaborative projects, liaising with academic collaborators.</p>	5%

## Person specification

	<b>Essential</b>	<b>Desirable</b>
<b>Skills</b>	<ul style="list-style-type: none"> <li>▪ Excellent oral and written communication skills, including the ability to communicate complex scientific concepts in publications and presentations to internal, national and international audiences.</li> <li>▪ Proven ability to creatively apply theoretical and computational methods to chemical and solid state physics problems.</li> <li>▪ Ability to play a leading role within a multidisciplinary team in the development of new research directions and managing collaborations with external partners.</li> <li>▪ Ability to use a range of software packages such as ORCA, QChem, CP2K and/ or GPAW.</li> </ul>	
<b>Knowledge and experience</b>	<ul style="list-style-type: none"> <li>▪ Demonstrated track record of excellence in theoretical and computational chemistry with publications in peer-reviewed journals.</li> <li>▪ Proven track record in quantum chemical method development spanning both wavefunction and density functional theories, including to model the effects of magnetic fields.</li> <li>▪ Demonstrated experience in applying theoretical and computational approaches to the study of both molecular and solid state systems.</li> </ul> <p>Experience in drafting research proposals for submission to external funding agencies.</p>	<ul style="list-style-type: none"> <li>▪ Experience in programming using one or more of the following languages: C, C++, Fortran 77/90/03, Python.</li> </ul> <p>Experience in applying quantum chemical approaches to investigate quantum sensing platforms.</p>
<b>Qualifications, certification and training (relevant to role)</b>	PhD or equivalent in theoretical / computational chemistry or theoretical physics, OR near to completion of such a PhD.	



The University of Nottingham is focused on embedding equality, diversity and inclusion in all that we do. As part of this, we welcome a diverse population to join our work force and therefore encourage applicants from all communities, particularly those with protected characteristics under the Equality Act 2010.

## Expectations and behaviours

The University has developed a clear set of core expectations and behaviours that our people should be demonstrating in their work, and as ambassadors of the University's strategy, vision and values. The following are essential to the role:

- Valuing people** Is friendly, engaging and receptive, putting others at ease. Actively listens to others and goes out of way to ensure people feel valued, developed and supported.
- Taking ownership** Is clear on what needs to be done encouraging others to take ownership. Takes action when required, being mindful of important aspects such as Health & Safety, Equality, Diversity & Inclusion, and other considerations.
- Forward thinking** Drives the development, sharing and implementation of new ideas and improvements to support strategic objectives. Engages others in the improvement process.
- Professional pride** Is professional in approach and style, setting an example to others; strives to demonstrate excellence through development of self, others and effective working practices.
- Always inclusive** Builds effective working relationships, recognising and including the contribution of others; promotes inclusion and inclusive practices within own work area.

## Key relationships with others

