**ROLE PROFILE**

**Job Title:** Research Fellow (Title will be ‘Research Associate’ where an appointment is made before PhD is completed)

**School/Department:** School of Chemistry

**Job Family and Level:** Research and Teaching Level 4  
(Assignment will be Level 4 Career training grade where an appointment is made before PhD has been completed)

**Contract Status:** This post is available immediately, with a negotiable starting date and will be offered on a fixed-term contract for a period of three years.

**Hours of Work:** Full time, 36¼ hours per week

**Location:** School of Chemistry, University of Nottingham, University Park, Nottingham NG7 2RD

**Reporting to:** Dr. Andy Teale

**Purpose of the Role:**

The purpose of this role is to carry out research to develop new computational techniques for the simulation of molecular systems and materials. The person appointed will form part of a team of researchers working on the topDFT project ([https://cordis.europa.eu/project/rcn/213780_en.html](https://cordis.europa.eu/project/rcn/213780_en.html)), which aims to develop new approaches to treat the exchange-correlation problem within density-functional theories.

The person appointed will be expected to plan and conduct a programme of research in this area, making use of extensive high performance computing resources. They will also be responsible for writing up their work for publication.

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.

**Main Responsibilities**

1. To carry out research in order to develop new computational approaches in the context of the ERC funded topDFT project ([https://cordis.europa.eu/project/rcn/213780_en.html](https://cordis.europa.eu/project/rcn/213780_en.html)). This will include activities from:

   - Development of new perspectives on the exchange-correlation problem in density-functional theory (DFT); including new descriptions of the correlation energy via the electronic kinetic energy.

   - Development of a topological approach to DFT; including the development of new exchange-correlation methods and tools for decomposition of molecular systems according to the topology of their electron density.

   - Investigation of extensions of these methods to treat systems in the presence of strong electromagnetic fields; including development of new current-dependent DFT methods and the treatment of non-collinear magnetism.
2. Write high quality scientific articles.

3. Give presentations internally at group meetings and externally at national and international conferences.

4. Liaise with academic collaborators as appropriate and identify and develop opportunities for research grant funding proposals.

5. To co-supervise undergraduate and/or postgraduate students projects, as appropriate. To participate in the assessment of student knowledge and co-supervise projects at Masters level.

6. You may be asked to perform other duties occasionally which are not included in the above but appropriate to the grade and consistent with the role.

7. To utilise and contribute to organising research resources and facilities, as appropriate.

### Knowledge, Skills, Qualifications & Experience

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<tr>
<th>Qualifications/ Education</th>
<th>Essential</th>
<th>Desirable</th>
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<tr>
<td><strong>Education</strong></td>
<td>Demonstrate excellence in theoretical and computational chemistry.</td>
<td>Established reputation for research in computational chemistry/physics/materials.</td>
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<td>PhD or equivalent in computational / theoretical chemistry or theoretical physics OR near to completion of a PhD.</td>
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<td><strong>Skills/Training</strong></td>
<td>Excellent oral and written communication skills, including the ability to communicate complex information with clarity.</td>
<td>Ability to play a leading role in research group in developing independent research pathways.</td>
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<td>Ability to creatively apply relevant research approaches, models, techniques and methods.</td>
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<td><strong>Experience</strong></td>
<td>A good publication record in international peer-reviewed journals commensurate with stage of career.</td>
<td>Experience in programming in one of the following languages; C, C++, Fortran 77/90/2003, Python.</td>
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<td>Experience in (co)supervision research students.</td>
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<td>Experience in the development of new computational methods in computational chemistry.</td>
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| Statutory/Legal | To take reasonable care for the health and safety of yourself and of other persons who may be affected by your acts or omissions at work in accordance with the Health and Safety at Work Act 1974, EC directives and the University’s Safety, Health and Environment Policies and procedures and to cooperate with the University on any legal duties placed on it as the employer. |

The University of Nottingham strongly endorses Athena SWAN principles, with commitment from all levels of the organisation in furthering women’s careers. It is our mission to ensure equal opportunity, best working practices and fair policies for all.