

# **Candidate Information**

Position:	Research Fellow
School/Department:	School of Mathematics and Physics
Reference:	25/112621
Closing Date:	Monday 23 June 2025
Salary:	£39,922 - £41,112 per annum
Anticipated Interview Date:	Thursday 10 July 2025
Duration:	1 year

## JOB PURPOSE:

The Research Fellow will be a key member the antimatter and many-body physics research group of Dermot Green (https://blogs.qub.ac.uk/antimatter/members/). The primary responsibility will be to develop many-body theory and its computational implementation for positron interactions with atoms, molecules and condensed matter, helping to deliver the aims of the ERC Consolidator Grant "ANTIMATTER". The Research Fellow will develop many-body theory and its computational implementation on high-performance computing clusters to enable ab initio calculations of positron-molecule scattering and for positron interactions in condensed matter, specifically adapting the group's MPI-parallelised C/C++ code EXCITON+. Depending on the expertise of the candidates, development of ab initio approaches (e.g., QED coupled cluster) to calculate processes involving molecules in optical cavities can also be considered.

The Research Fellow will be expected to conduct independent and collaborative research as directed by the PI, prepare results for publication in leading scientific journals, and present at national/international conferences and workshops. The role also includes engagement with the wider research team at QUB and with our international collaborators, including by contributing to collaborative software development, and, where appropriate, mentoring junior researchers/undergraduate research project students.

#### **MAJOR DUTIES:**

- 1. Develop many-body theory and its computational implementation for positron interactions with atoms, molecules and condensed matter, helping to deliver the aims of the ERC Consolidator Grant "ANTIMATTER".
- 2. Develop the group's EXCITON+ C code and perform calculations on Tier-2 and national/international supercomputing clusters.
- 3. Carry out analyses, critical evaluations, and interpretations of calculated data and comparisons of it with experiment and other theoretical methods.
- 4. Produce high quality research outputs consistent with project aims and commensurate with career stage. This will include collaborating and co-authoring with PI and project team (as appropriate) on outputs.
- 5. Present at national and international conferences.
- 6. Assist grant holder in the preparation of funding proposals and applications to external bodies.
- 7. Carry out occasional educational supervision, demonstrating or lecturing duties within the post holder's area of expertise and under the direct guidance of a member of academic staff.
- 8. Undertake supplementary duties relevant to the success of the project including administrative duties and additional training and development activities as required.

#### **ESSENTIAL CRITERIA:**

 Have a PhD or be about to obtain a PhD\* in theoretical atomic, molecular physics or quantum chemistry including many-body theory (one of diagrammatic many-body theory; diagrammatic Monte Carlo, or coupled cluster theory) and its computational implementation for atoms/molecules and/or condensed matter. (\*must by application deadline have submitted thesis and have successfully defended viva). 2. Specific, relevant\* research experience to include:

• Previous research experience (including PhD duration) as evidenced by preprints/publications and/or by a completed PhD thesis in either:

(i) theory of low-energy positron/positronium interactions with matter, and/or

(ii) theory of low-energy electron-matter interactions, including theory and calculations of electronic structure, scattering, interatomic Coulomb decay/electron capture, or ab initio QED calculations of light-matter interactions involving atoms and molecules in optical cavities.

• Track record (demonstrated via PhD thesis/preprints or journal articles) in high-performance scientific computing for theoretical physics and/or chemistry, specifically in using and/or developing parallelised codes (preferably in C/C++ language) and its use on high-performance computing clusters

- 3. Track record of working collaboratively within a research team environment, including providing research support to other researchers and undergraduate project students.
- 4. Proactive and self-motivated, with the ability to work independently, manage time effectively, and take initiative in driving research forward.
- 5. Strong communication skills, both written and oral, with the ability to explain complex theoretical concepts clearly to diverse audiences, including experimental collaborators or non-specialists.
- 6. Commitment to continuous professional development.
- 7. Ability to start July 2025 (or as soon as possible thereafter).

## DESIRABLE CRITERIA:

- 1. Hold a 1st-class masters level undergraduate degree in either physics, theoretical physics, applied mathematics, quantum chemistry, or suitably related field.
- 2. Previous experience in quantum many-body theory calculations for electron/positron scattering on atoms/molecules (i.e., solving Lippmann-Schwinger equation via T-matrix or Schwinger variational methods).
- 3. Experience in GW (or alternative diagrammatic) calculations for electronic structure calculations for atoms/molecules and/or condensed matter.
- 4. Experience of calculating positron annihilation rates and annihilation gamma spectra for atoms and/or molecules.
- 5. Experience developing and using Gaussian-basis electronic structure codes (e.g., EXCITON+, Gaussian, GAMESS etc) for quantum chemistry/computational electronic structure/processes of atoms and/or molecules.
- 6. Experience developing and using Gaussian-basis electronic structure codes (e.g., EXCITON+, Gaussian, GAMESS etc) for quantum chemistry/computational electronic structure/processes of condensed matter.
- 7. Experience developing ab initio approaches for light-matter coupling for atoms and/or molecules in optical cavities, e.g., QED Hartree Fock and QED coupled-cluster theory.