PhD in Theoretical many-body physics and quantum chemistry:
Many-body theory and computation of low-energy antimatter interactions with matter and light [within ERC-funded research group].

Funded: Two positions available; one for international applicants (covering international fees and stipend) and one UK/ROI-based applicant.
Duration: 3.5 years (possibly 4).
Start Date: 1st October 2026 (earlier could be considered).

Project summary:

The project will contribute to Prof Green's ERC Consolidator Grant project, by developing state-of-the-art methods in theoretical and computational atomic, molecular and condensed matter physics, chiefly to describe the fundamental quantum mechanical interactions of antimatter (positrons and positronium) with matter.

Positrons are the antiparticles of electrons. They are routinely trapped, accumulated and delivered in beams for studies of fundamental, atomic and molecular physics, and have important uses in materials science (as ultrasenstive diagnostics of defects and porosity in materials), in medical imaging (in positron-emission tomography) and astrophysics (in understanding the molecular composition of the installer medium, detecting neutron/black-hole mergers, and theories of dark matter etc).

Positron and positronium interactions with atoms, molecules and condensed matter are characterised by strong many-body correlations. They have an overwhelming effect, modifying scattering cross sections, enhancing annihilation rates, and enabling and enhancing positron binding. They also make the theoretical description a challenging many-body problem. The theoretical description of positronium interactions with atoms and molecules is more challenging still, owing to the composite nature of the projectile and target, and the delicate balance of exchange interaction, van der Waals attraction and many-body correlations. It is of current interest, motivated by intensive ongoing developments of the new JPET positronium-based medical imaging device, and the recent prediction of positronium-dissociative attachment.

Our group [group website: https://blogs.qub.ac.uk/antimatter/] has made groundbreaking progress recently, developing ab initio methods to describe low-energy positron interactions with molecules, as reported in e.g., *Nature* https://www.nature.com/articles/s41586-022-04703-3 and highlighted in *The Irish Times* https://www.irishtimes.com/science/space/2022/06/25/antimatter-mystery-solved-by-physicists-at-queens-university-belfast-and-trinity-college/.

There are numerous directions in which the PhD research could progress, including developing our EXCITON+ code to enable new calculations of positron binding, scattering and annihilation in atoms and molecules, positronium-molecule interactions, positron interactions in condensed matter, or development of new methodologies including positron-coupled-cluster theory (which may provide a formalism to describe antimatter interactions with molecules whose electronic structure is tuneable via their coupling to light) and diagrammatic Monte Carlo (the numerical summation of Feynman diagram series via stochastic sampling). It will involve

developing our in-house scientific software that run on high-performance computing systems.

The research programme is funded by a European Research Council Consolidator grant and it is anticipated that the PhD student(s) will join a group of multiple Research Fellows and other PhD students working on synergistic problems and providing a stimulating environment. Collaboration is anticipated with experimental groups including the pioneering University California San Diego positron group, and with pre-eminent theorists and high-performance computing experts in Imperial, NTNU Norway, Heidelberg, etc.

The applicant should have a background and interest in any of quantum mechanics/quantum field theory/theoretical or computational physics and chemistry (including e.g., many-body theory/coupled-cluster theory), or computer science. Please contact Prof. Green if in doubt.

Recent publications by PhD students in our group:

1. J. Hofierka, ..., D. G. Green, Nature **606**, 688 (2022) https://www.nature.com/articles/s41586-022-04703-3

2. J. Cassidy, ..., D. G. Green *"Many-body theory calculations of positron binding to halogenated hydrocarbons",* Phys. Rev. A **109** Letter 040801 (2024) https://doi.org/10.1103/PhysRevA.109.L040801

3. J. Cassidy, ..., D. G. Green, "Many-body theory calculations of positronic-bonded molecular dianions", J. Chem. Phys. Emerging Investigator Special Annual Collection (2024); Editor's featured article] https://doi.org/10.1063/5.0188719.

4. A. Baidoo, ..., D. G. Green, *"Positron annihilation and binding in aromatic and other ring molecules",* Phys. Rev. A **109**, 062801 (2024). [Editors' suggestion]

5. C. M. Rawlins,..., D. G. Green, *"Many-Body Theory Calculations of Positron Scattering and Annihilation in molecular hydrogen, nitrogen and methane",* Phys. Rev. Lett. **130**, 263001 (2022).

Group website: https://blogs.qub.ac.uk/antimatter/