

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: funding from ERC.

Duration: 3 years (possibly 4).

Start Date: 1st October 2025.

Project summary:

The project will develop 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 ultrasensitive diagnostics of defects and porosity in materials), in medical imaging (in positron-emission tomography) and astrophysics (in understanding the molecular composition of the interstellar medium, detecting neutron/black-hole mergers, and theories of dark matter etc).

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, or 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. It will involve running and developing our codes 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 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.

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/>