# PhD Studentship in Computational Chemistry of Graphene-Based Materials

School of Chemistry, University of Birmingham          Supervisor: Prof. Ganna (Anya) Gryn'ova

## Details

A fully funded UK home rate) 3.5-year PhD position is available in the Computational Carbon Chemistry group of Prof. Ganna (Anya) Gryn'ova (School of Chemistry, University of Birmingham) to work on the computational modelling of graphene and its derivatives. Tentative starting date for this position is **April 2024** (negotiable).

Background. Graphene and its derivatives have arisen in recent years as an attractive alternative to silicon and transition metal-based materials for efficient and sustainable carbocatalysis and energy conversion. Numerous advantages of graphene-based materials include their biocompatibility, structural variability, mechanical flexibility, unique electronic and optical properties, ease of fabrication and functionalisation, and inherent molecular nature. Despite many developments in this enticing field, lack of an in-depth understanding of the associated chemistry impedes its transition from empirical serendipity to rational, practice-oriented design. The goals of this project are to elucidate the key chemical factors determining the efficiency of GBMs across diverse practical applications and design new graphene-based functional materials.

Project. This research project will involve investigating the chemistry of GBMs relevant to their applications as (*i*) carbocatalysts, (*ii*) electrocatalysts, and (*ii*) hybrid electrode materials. You will work in close cooperation with other group members working on multiscale materials modelling and focussing on other types of functional organic materials and build upon our recent developments in this area. You will receive an in-depth training in a range of computational chemistry techniques, from highly accurate electronic structure theory to multiscale approaches. You will acquire expertise in the cutting-edge field of graphene-based materials, which, together with the acquired technical proficiencies, will equip you with a competitive professional profile for both academia and industry. You will also receive training in diverse transferable skills.

Research environment. The Computational Carbon Chemistry group, led by Anya Gryn'ova, started in 2019 in Heidelberg, Germany (https://www.h-its.org/research/ccc/); today, our dynamic team includes undergraduate and PhD students and postdocs coming from diverse backgrounds and nationalities but united in our love of chemistry, computers, and [nerdy] banter over coffee. In April 2024, the group will relocate to UK and join the rapidly growing computational chemistry section at the School of Chemistry, University of Birmingham. The University of Birmingham was founded in 1900 on an anti-discrimination ethos and remains committed to promoting equality, diversity, and fairness. Moreover, the School of Chemistry holds an Athena SWAN Bronze Award, which recognises its work in promoting women's careers in science, technology, engineering, mathematics and medicine (STEM).

Qualifications. Successful candidates should have or expect to soon receive a first or upper second (2.1) honours degree (or equivalent) at a Bachelor's or Master's level in chemistry, physics, materials science, or a related discipline. Experience in theoretical/computational chemistry, numerical simulations, and/or materials science, as well as basic programming skills are desirable.

Funding Notes. This studentship is fully funded for 3.5 years and includes a tax-free annual stipend and fees at the UK home rate. Additional funding will be available to cover research and training costs, conference attendance, etc. Due to funding restrictions, applicants not eligible for UK home fee status will only be considered if they can secure additional external funding to cover international fees.

## How to Apply

To apply, please send the following as a single PDF attachment *via* **email to Prof. Ganna (Anya) Gryn'ova (g.grynova@bham.ac.uk)**: (1) a cover letter (1 page max.) indicating your earliest starting date; (2) a full curriculum vitae; (3) a transcript listing courses taken and grades received; (4) contact details of two referees. Applications will be accepted **until 1 March 2024**, but the position will be filled as soon as an appropriate candidate is found.