



## PhD Studentship in Computational Materials Chemistry and Machine Learning

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 to work on the intersection of computational materials science and chemical machine learning. Tentative starting date for this position is **July 2026** (flexible and negotiable).

Background. Functional, topologically complex organic molecules are rising stars in modern materials science due to their biocompatibility, structural variability, and wealth of physico-chemical properties. Our group uses theoretical and computational chemistry, physics, and materials science in combination with chemical machine learning to explore and exploit diverse functional organic and hybrid materials and molecules. We are particularly interested in *graphene*-based materials, *covalent-organic frameworks* and *cages*, and *hyperbranched polymers* in the context of their applications in capture, storage, transport, and/or catalytic transformations of therapeutic molecules and environmental pollutants.

Project. This position allows adaptive approach to the central topic of the PhD depending on your background and interests. Possible research directions include constructing *multiscale simulation workflows* and applying them to *materials design*, and/or developing and implementing novel *machine learning representations* for functional organic materials. You will work in close cooperation with other group members and receive an in-depth training in a range of simulation techniques and in various aspects of chemical machine learning. This position will equip you with a competitive professional profile and a range of transferrable skills for both academia and industry.

Research environment. The Computational Carbon Chemistry group (<https://www.grynova-ccc.org/>), led by Anya Gryn'ova, 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. The group is part of the dynamic 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, computer science, or a related discipline. Experience in theoretical/computational chemistry, numerical simulations, materials science, and/or data science is 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 13 April 2026**, but the position will be filled as soon as an appropriate candidate is found.