



Postdoc Position in Computational Materials Chemistry

School of Chemistry, University of Birmingham

Supervisor: Prof. Ganna (Anya) Gryn'ova

Details

A full-time 2-year postdoctoral position is available in the Computational Carbon Chemistry group of Prof. Ganna (Anya) Gryn'ova to work on the ERC Starting Grant "PATTERNCHEM: Shape and Topology as Descriptors of Chemical and Physical Properties in Functional Organic Materials". Tentative starting date for this position is **April 2024** (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. In PATTERNCHEM, several families of functional organic materials – graphenes, covalent-organic frameworks, and hyperbranched polymers – are investigated through a combination of high-level quantum chemistry, multiscale materials simulations, and interpretable machine learning. The ultimate goal of PATTERNCHEM is to build an all-encompassing, adaptable framework for modelling interactions of multifaceted functional organic materials with their molecular targets, filling the missing links with newly devised structural fingerprints and energetic descriptors.

Project. This interdisciplinary research project will involve high-level, high-throughput, and multiscale simulations of functional organic materials, including graphene derivatives, covalent organic frameworks, and hyperbranched polymers, as well as implementation of these methods into automated computational workflows and generation of diverse material datasets. You will work in close cooperation with other group members working on PATTERNCHEM and chemical machine learning. You will acquire expertise in the cutting-edge field of functional organic materials, which will equip you with a competitive professional profile for both academia and industry. You will also receive training in diverse transferable skills and mentorship regarding future career pathways.

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 a PhD degree (or be close to completion) in chemistry, physics, materials science, or a related discipline, and an experience in theoretical/computational chemistry/materials science and numerical simulations. Expertise in high-throughput and multiscale simulations, automated computational workflows, data science, as well as programming is desirable.

Salary and Contract. Full time starting salary (Grade 7) is normally in the range of £34,980 to £44,263 per annum, with potential progression once in post to £46,974. This is a fixed-term 2-year contract up to May 2027 depending on the start date.

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 list of publications; (4) contact details of two referees. Applications will be accepted **until 15 March 2024**, but the position will be filled as soon as an appropriate candidate is found.