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 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 (*i*) developing and implementing novel machine learning representations and fingerprints of shapes and topologies for functional organic materials, and (*ii*) modelling host-guest interactions in hyperbranched polymers. You will work in close cooperation with other group members working on PATTERNCHEM and chemical machine learning. You will receive an in-depth training in a range of simulation techniques and in various aspects of 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.

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, materials science, and/or data science, as well as programming 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 1 March 2024**, but the position will be filled as soon as an appropriate candidate is found.