DESCRIBING CHEMICAL SIMULATION WITH A BAYESIAN WORLDVIEW

Analysis of experimental techniques is becoming increasingly reliant on computational chemical simulations. However, our simulations often fail to cover experimental timescales, meaning that we often extrapolate our conclusions in the hope that our simulations represent the real system. A Bayesian approach, where we propose a probabilistic model to describe our system (based on the underlying physics and chemistry), should improve the comparison between simulation and experiment [1]. In this project, you will develop probabilistic models for chemical systems and apply these models in a range of areas.

The analysis of experimental data, such as X-ray diffraction and neutron scattering, the generation of machine learning models and the use of quantum computing algorithms can all benefit from such probabilistic models. You will have the opportunity to pursue areas of your own academic interest in the applications of these mathematical models.

This PhD project will be based in the SCAMs@bristol research group (scams-research.github.io) at the University of Bristol School of Chemistry under the supervision of Dr Andrew McCluskey. In SCAMs@bristol, we are interested in developing physics-informed analysis methods and investigating how these methods can be used to improve chemical data analysis and discover new materials. In addition to learning valuable computational chemistry and mathematical modelling skills, you will develop substantial programming, software engineering, and data science experience and be encouraged to explore your research interests. There will also be opportunities to collaborate with experimental colleagues from large-scale neutron and X-ray scattering facilities, such as Diamond Light Source, ISIS Neutron and Muon Source and the European Spallation Source.

The successful candidate will be curious and excited to apply novel mathematical methods to physical systems and should hold (or be predicted to achieve) a First or Upper Second class degree in Chemistry, Physics, Chemical Physics or a related area. The 3.5 year PhD studentship, for a September 2024 start, is fully funded with a stipend to cover living costs at the level set by UKRI, for UK applicants and EU citizens with settled status (international students may be eligible to apply for a University of Bristol PGR Scholarship). Interested applicants are invited to contact Dr Andrew McCluskey (andrew.mccluskey@bristol.ac.uk) for further details.

References

[1] McCluskey, AR, Coles, SW, & Morgan, BJ, *arXiv*, 2305.18244 (2023), doi:10.48550/arxiv.2305.18244.