Molecular Modeling for Design of Biochar Materials

A PhD studentship is available in the groups of Dr Valentina Erastova at the School of Chemistry and Dr Ondrej Mašek at the School of Geosciences, the University of Edinburgh.

The studentship is fully-funded for 42 month (incl stipend starting at £15,009 per annum) and is part of the E4 Doctoral Training Partnership. See Funding and Eligibility: www.ed.ac.uk/e4-dtp/how-to-apply/funding-and-eligibility

Project Summary
The project brings molecular modeling into biochar research, providing atomistic details to the key properties of biochar, and through this enabling the informed design and optimization of biochar for desirable functionality.

Background
Biochar is a low-cost environmental carbon-rich porous material produced through pyrolysis of biomass, a waste organic material resulting from diverse human activities. Depending on the biomass composition and production conditions, biochar will express a range of physical and chemical properties, tunable to suit many applications. Examples of its use can be found in water conservation and desalination, pollution remediation, heavy metal sequestration, carbon dioxide capture, and soil nutrient management. A full understanding of the mechanisms behind biochar functionality is critical for the targeted design and optimisation of its properties, currently obtained through trial-and-error.

Molecular dynamics (MD) is a modelling technique providing atomic-level insights into physicochemical interactions. Here, MD is of a particular use to characterise energetics and dynamics of the adsorption and release processes occurring between biochar surfaces and adsorbate (metal ions, pollutants, nutrients, gasses). Modelling delivers key descriptors behind behaviours observed in laboratory and field experiments. Furthermore, MD allows us to design and test hypothetical biochar models, aiming at desired functionality, prior to engaging in biochar production for its successful modification.

Biochar is a complex system, and to date there is no realistic model of it. The aim of this project is to create a tool for generating realistic biochar models ready for MD simulations, based upon analytical insights (exposed surfaces, interlinking, porosity, functional groups, their surface density, etc). This tool will allow scientists without strong computing backgrounds to perform theoretical studies of systems of interest. Overall, the project is a key steppingstone to bringing molecular modelling to the extensive biochar research community, enabling scientists to better understand and design this important material.

AIM 1: Create the first realistic molecular model of biochar guided by experimental observables.
AIM 2: Leveraging molecular simulation, rationalize interactions within biochar and guide design for specific applications:
- What physicochemical characteristic of biochar determines its property?
- How can we modify its physicochemical structure for optimal performance under given environmental conditions?
**Full Project Description** → [www.ed.ac.uk/e4-dtp/how-to-apply/our-projects?item=849](http://www.ed.ac.uk/e4-dtp/how-to-apply/our-projects?item=849)

Further information about the E4 DTP [www.ed.ac.uk/e4-dtp](http://www.ed.ac.uk/e4-dtp)

More information about research in the group, see [www.erastova.xyz](http://www.erastova.xyz)

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**Application Deadline:** 9th of January 2020, 12 noon

Please follow this link to apply [www.ed.ac.uk/e4-dtp/how-to-apply](http://www.ed.ac.uk/e4-dtp/how-to-apply)

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