PhD position at the University of Liverpool, United Kingdom.

Title : Analysis of energy landscapes of molecular crystal structures employing combinatorial and topological methodologies.

Deadline : 1 May 2018, funded for 3 years from October 2018 by the Leverhulme Research Centre for Functional Materials Design.

Eligibility : UK/EU, international students can pay higher tuition fees.

Supervisors : Dr Yannis Goulermas, Dr Vitaliy Kurlin, Prof Graeme Day.

Description. This is an opportunity for an exciting cross-disciplinary project at the interface between computer science, mathematics and materials chemistry at the Materials Innovation Factory. The work will involve the development of novel combinatorial and topological modelling and optimisation concepts for applications in chemistry. The models will be used to study crystal structure energy landscapes whose understanding requires an efficient search by combinatorial optimisation algorithms; the results of these calculations are used to guide the discovery of new, functional materials. These models will also be generically applicable to problems, such as modelling data knowledge and large-scale data visualisation, object ordering and graph matching. The supervisory team has a strong track record in the defining ingredients of the underlying work and will closely contribute to the research. Publications in top-tier theoretical and application-oriented venues will be expected.

Requirements. The candidate should have at least a 2.1 BSc in Computer Science, Mathematics or related discipline, be proficient with linear algebra and calculus, knowledgeable in discrete and continuous optimisation methods, and also competent in computer programming (Matlab, R, Python, or C++).

Informal enquiries : Dr Vitaliy Kurlin, e-mail vitaliy.kurlin@gmail.com.

Application link : https://www.findaphd.com/search/ProjectDetails.aspx?PJID=9381