

PhD position at the [University of Liverpool](#), United Kingdom.

Title : Data Driven Discovery of Functional Molecular Co-crystals.

Deadline : 31 July 2018 (an earlier offer can be made to a strong candidate), funded for 3.5 years from October 2018 by [Leverhulme Research Centre for Functional Materials Design](#) and [Cambridge Crystallographic Data Centre](#).

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

Supervisors : Dr [Matthew Dyer](#) and Dr [Vitaliy Kurlin](#).

Description. We propose to use the information stored within the [Cambridge Structural Database](#) (CSD) to identify the best molecular candidates to form co-crystals with fullerides and polyaromatic hydrocarbons (PAHs). Although few co-crystals involving fullerides and PAHs have been reported, there are many more co-crystals in the database which contain information about which pairs of molecules do form co-crystals together. The first step is to design a geometric code that is invariant under all rigid motions in and uniquely represents any periodic co-crystal structure. The second step is to define a similarity measure between resulting codes. The third step is to apply [Topological Data Analysis](#) for build a topological map of all existing co-crystals from the CSD. The fourth step is to use Machine Learning on a smaller subset of known co-crystals with good properties in this map as a guide for searching new co-crystals with better properties. As well as crystal structures, the CSD will also provide molecular identifiers of the molecules in co-crystals (e.g. InChI, SMILES). These will be used to compute descriptors and measures of molecular similarity commonly used in pharmaceutical research, which in turn become features in machine learning and data science algorithms..

Environment : [Materials Innovation Factory](#).

Requirements. Applications are welcomed from students with a 2:1 or higher masters degree or equivalent in Computer Science or Chemistry, particularly those with the skills relevant to the project outlined above.

Programmings skills : C++ or Python.

Informal enquiries : Dr [Vitaliy Kurlin](#), e-mail vitaliy.kurlin@gmail.com.

Application link : <https://www.findaphd.com/search/ProjectDetails.aspx?PJID=9114>