Applications are invited for a three-year PhD studentship on quantum mechanical simulations of organic electronics, available at Imperial College London starting in October 2018.

Organic semiconductors have many properties which are not only ideal for existing electronic devices such as organic light emitting diodes (OLEDs) and solar cells, but which could also lead to new technologies which cannot be realized with inorganic materials. However, there is a need to improve aspects such as device efficiency. Computer modelling has an important role to play, first for understanding the underlying physical processes and ultimately as a predictive tool. However, these materials are challenging to simulate using quantum mechanics (QM), as calculations of thousands of atoms are required to capture their disordered structure. This is beyond the capability of most existing QM models even when using supercomputers; there is therefore a need to develop software which can treat large systems without compromising on accuracy.

In this PhD project you will develop and apply QM methods for modelling organic electronics, focussing on materials for OLEDs. You will use methods based on density functional theory (DFT) and will exploit techniques for large systems, including linear-scaling DFT and multi-scale approaches, as well as methods for excited states. You will implement your developments in the open source BigDFT code, and will run simulations on parallel supercomputers. You will be a part of the Thomas Young Centre for Theory and Simulation of Materials and will collaborate with other researchers with expertise in modelling and experiment, who are based in the UK and internationally.

We encourage informal enquiries about the project, which can be made to Dr. Laura Ratcliff at laura.ratcliff08@imperial.ac.uk. Further information on the area of research, including relevant publications, can be found at https://www.imperial.ac.uk/people/laura.ratcliff08.

Applicants should have a Master’s degree or First degree or (equivalent) with First Class or Upper Second Class in Physics, Chemistry or Materials Science, a strong interest in materials modelling and high performance computing, and experience with computer programming.

This PhD studentship is funded by the UK's Engineering and Physical Sciences Research Council and is open to UK home students or European students who have spent the last three years in the UK. The studentship will cover tuition fees plus the standard maintenance stipend of £16,553 (this year’s rate) per annum.

Applicants should send a CV and covering letter to Dr. Laura Ratcliff at laura.ratcliff08@imperial.ac.uk and will be required to complete an electronic application form. The prospectus, entry requirements and application form (under 'how to apply') are available at: http://www.imperial.ac.uk/pgprospectus. Please contact Fiona Thomson (fiona.thomson@imperial.ac.uk) for further information. Information about the Department can be found at http://www3.imperial.ac.uk/materials.

Closing date: a month from placement (Midnight BST)

Committed to equality and valuing diversity, we are also an Athena SWAN Silver Award winner, a Stonewall Diversity Champion, a Disability Confident Employer and are working in partnership with Gires to promote respect for trans people.

The College is a proud signatory to the San-Francisco Declaration on Research Assessment (DORA), which means that in hiring and promotion decisions, we evaluate applicants on the quality of their work, not the journal impact factor where it is published. For more information, see https://www.imperial.ac.uk/research-and-innovation/about-imperial-research/research-evaluation/