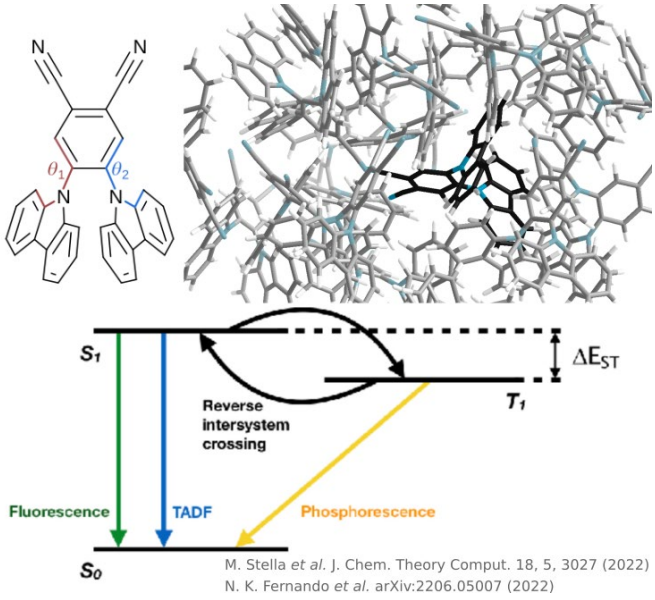
Simulating Next Generation Organic Light Emitting Diodes



About the project or challenge area: Organic semiconductors have a number of advantages for use in devices such as light emitting diodes (LEDs), including light weight, low cost and flexibility. However, the current generation of organic LEDs (OLEDs) are based on molecules containing scarce and expensive heavy metals such as Ir and Pt, motivating the development of OLEDs based on molecules exhibiting thermally activated delayed fluorescence (TADF). TADF-based emitters can be purely organic, avoiding the need for heavy metals and leading to efficient and environmentally-friendly devices. Given the vast number of potential TADF emitters, computational chemistry has an important role to play in identifying new TADF molecules, for example by calculating key properties which govern TADF, such as the singlet-triplet splitting. However, this is complicated by the need to account for factors such as disorder and environmental effects, which can have a strong influence on properties. This project will use density functional theory to simulate TADF-based emitters, with the aim of providing new insights into their electronic structure.

Why choose this opportunity? The focus of your project will be on using computational chemistry to simulate TADF-based OLEDs, which will provide an excellent platform to learn about the use of computational chemistry for practical applications. Your work in this area can make a real impact on global challenges, such as the development of emitters for environmentally friendly OLEDs. You will develop and increase your expertise in computational chemistry and coding, whilst becoming familiar with the fundamentals of electronic structure. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge required to understand concepts related to electronic structure, as well as an enthusiasm for computational research and coding, and teamwork and time management.

Bench fees: A bench fee of £2500 is required.

How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Laura Ratcliff, Research Fellow in the School of Chemistry. You can contact her at laura.ratcliff@bristol.ac.uk

Find out more about your prospective research program: *High-efficiency organic light-emitting diodes from delayed fluorescence,* Nature **492**, 234 (2012), https://www.nature.com/articles/nature11687