PhD Scholarship: Computational investigation of 2D carbon nitride photocatalysts for H_2 production

Project description: Accelerating climate change and future energy crises mean we need an urgent transition to a low-carbon economy. H_2 fuel will be a key component of our future energy needs, but at present the majority of H_2 production relies on fossil fuels. Photocatalytic processes that utilise solar energy to facilitate water splitting to H_2 and O_2 gas have considerable potential to provide clean H_2. Non-toxic, abundant materials can be used in the catalytic process, for which C_3N_4 is a promising candidate.

To realise the potential of C_3N_4 as a photocatalyst for H_2 production, several questions need to be addressed. The catalytic process itself is not well understood in terms of the energetics, where the active sites are and how charge transfer is facilitated. The structures of the C_3N_4 material, its interaction with host materials and incorporation of dopants, as well as the presence of defects, need to be investigated. First principles calculations can provide crucial insights and help answer these questions in ways that are not possible with experimental techniques. However, this project will require close collaboration with experimentalists working on designing these photocatalytic systems. Such detailed calculations are severely lacking at present.

This project aims to investigate thoroughly the photocatalytic properties of graphitic C_3N_4 using first principles calculations and theoretical development. You will join a dynamic team and collaborate closely with experimental groups with the School of Engineering. Both in-house and national supercomputing resources will be utilised throughout the project. The research goal is to gain a comprehensive understanding of the photocatalytic properties of graphitic C_3N_4, which will facilitate significantly more efficient and green hydrogen production.

The outcomes of this project for the PhD candidate are listed below:

- understand electronic structure of materials;
- learn computational methods to investigate the properties of materials;
- develop and apply physical models of photocatalytic processes on material surfaces;
- learn computer coding skills;
- analyse data using a variety of tools;
- understand key issues regarding hydrogen production;
- present findings at national and international conferences;
- publish high-quality research in appropriate journals.

This PhD is a School of Engineering Bursary covering fees and a £18k stipend per annum for three years. As part of the candidate's academic development, the bursary agreement includes that the successful PhD candidate engages in 4 hours per week student contact time, comprising lab class assistance and extracurricular activity development. If you have any informal query please email the supervision team directly. We encourage applications from underrepresented groups.

Supervisory Team: The successful applicant will work with Dr John Buckeridge (google scholar), an expert in computational materials physics whose research aims to understand the fundamental properties of a range of functional materials (https://jbuckeridge.github.io) and with Dr Suela Kellici (google scholar), an expert in chemical synthesis and green energy who runs the Nano2D Lab (www.nano2d.co.uk).