

Department of Physics & Department of Chemistry



Fully Funded PhD Studentships

Prof. Nicholas Hine & Dr. Sebastian Pike

PhD project: Electronic Structure & Photochemistry of Molecular Iron(III)-oxo Clusters

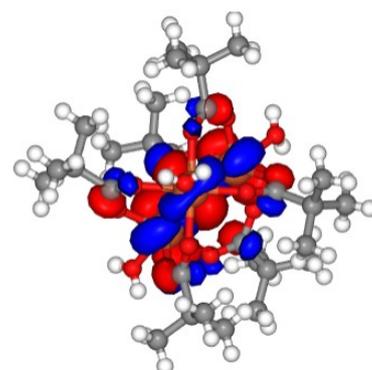
Supervisors: Prof. Nicholas Hine & Dr. Sebastian Pike

Key Dates: **Applications very much welcomed - the position remains open**

Project description:

A PhD studentship (3.5 years) funded by The Leverhulme Trust is available for a talented researcher with an interest in Theory and Simulation of Strongly-Correlated systems with applications to photochemistry and sustainable fuels.

α -Hematite (Fe_2O_3) is a leading material for sunlight driven water splitting, a process which converts solar energy into a chemical fuel. However, certain intrinsic limitations hinder its efficient use. Reducing the size of a hematite particle to the nanoscale can increase efficiency, however, this poses a fascinating question – how is the electronic structure and photochemistry of a strongly correlated metal oxide like hematite affected by particle size? This project will explore the electronic structure of Fe(III)-oxo clusters, which are well-defined molecules with precise but tuneable geometry, and are analogous to very small hematite particles. These studies will make important conceptual bridges between the fields of materials science and molecular chemistry and the findings will inspire design of new more efficient iron-based materials for solar energy harvesting.



The two PhD projects will progress in parallel, working independently but with regular contact as part of a wider research team. The students will benefit from a wide support network from both research groups and the opportunity to learn a wide range of skills.

The theory project will involve prediction and interpretation of the electronic structure, structure and dynamics of iron-oxo cluster molecules and understanding the nature of photochemical excitation in these systems. This PhD student will work in the Hine Group on a theory-focussed project, but will communicate and collaborate regularly with the experimental side of the project. Cutting-edge computational methods including linear scaling density functional theory, in combination with strong-correlation, theoretical

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spectroscopy and machine-learning approaches, will be developed and used to study these fascinating systems.

Both studentships have an associated travel budget for attending conferences/visiting collaborators and the opportunity to attend a specialised training school during the project.

Requirements:

Good degree (2.i or 1st class) in physics, chemistry, materials science or related subjects. Must be willing to work independently and as a key part of a research team. Funding is available for UK students only (overseas students are welcome to apply but would need to find additional funding for the full Band 2 Postgraduate Research fees (<https://warwick.ac.uk/services/academicoffice/finance/fees/pgr/>)).

How to apply:

In the first instance please contact Prof. Hine and/or Dr. Pike by email at <mailto:n.d.m.hine@warwick.ac.uk> and <mailto:sebastian.pike@warwick.ac.uk>. Please include in your email a CV and your current/predicted grades.

Research group information and more details of ongoing research is available here

<https://warwick.ac.uk/fac/sci/physics/staff/academic/nicholashine/>

<https://warwick.ac.uk/pikegroup/>

Details on how to apply formally can be found at <http://www.go.warwick.ac.uk/pgapply>