

Supervisor(s):

Dr Matthew Dyer msd30@liverpool.ac.uk

(Department of Chemistry, University of Liverpool, UK)

Dr Hsin-Yi Chen, Tiffany hsinyi.chen@mx.nthu.edu.tw

(Department of Engineering and System Science, National Tsing Hua University, Taiwan)

Project Title: DFT Computational Investigation into Perovskite Oxide Catalysts**Project Description:**

Catalysis is crucial for the function and performance of electrochemical devices (e.g. Lithium ion batteries, and fuel cells), and in the chemical industry's manufacture of products world-wide. The structure of the active surface of solid catalysts, and the mechanism of catalytic reactions occurring on them, are often complicated, but a good understanding of them is important in the generation of new improved catalysts. Computational studies, using atomistic methods such as density functional theory, can provide this level of understanding, often beyond that which can be gained from experiment alone.

The proposed studentship will focus on the computational modelling of a specific set of solid catalysts, mixed metal oxides with the perovskite structure. Initial research will focus on catalysts for the oxygen reduction reaction in solid oxide fuel cells. The student will seek to understand the role of different elements (Mo and W) in preventing the reaction of CO₂, when Mo and W are doped into the state of the art catalyst, Ba_{0.5}Sr_{0.5}Fe_{0.8}Co_{0.2}O_{3-d} (BSCF).

Several subsequent tasks are envisaged for research in the following years. For example:

1. Are any alternative elements also able to prohibit the formation of carbonate in BSCF?
2. What is the mechanism for O₂ reduction in Mo and W substituted BSCF.
3. Are there new interesting oxide catalysts with the perovskite structure which would be more timely targets of study.

The student will spend two years in NTHU under the supervision of Dr Chen, who has considerable experience in the field of computational heterogeneous catalysis, including CO₂ adsorption on oxide surfaces. In the following two years at the University of Liverpool, UK, the student will work with Dr Dyer applying this methodology on new catalysts. Dr Dyer has excellent links with experimental groups in Liverpool who are discovering new improved oxide catalysts, and with Johnson Matthey, an international company with special interest in heterogeneous catalysis.

A successful student will learn how to model solid catalysts with density functional theory, and in addition gain the necessary skills to pursue a career in scientific research.

Funding Notes:

This project is a part of a 4-year dual PhD programme between National Tsing Hua University (NTHU) in Taiwan and the University of Liverpool in England. It is planned that students will spend time studying in each institution.

Both the University of Liverpool and NTHU have agreed to waive the tuition fees for the duration of the project. Moreover, a stipend of TWD 10,000/month (approx. £265) will be provided as a contribution to living costs.

When applying please ensure you Quote the supervisor & project title you wish to apply for and note 'NTHU-UoL Dual Scholarship' when asked for details of how plan to finance your studies.