

## PhD Position - Design of Photocatalysts for CO<sub>2</sub> Activation

A PhD position is available at the Tyndall National Institute, University College Cork, under the supervision of Dr. Michael Nolan to work on first principles simulations in the design of new photocatalyst materials for CO<sub>2</sub> activation. The project **SuSChem Using theory-driven design to tailor novel nanocomposite oxides for solar fuel production**, funded under the Science Foundation Ireland US-Ireland R & D Partnership Program, in collaboration with University of Ulster and Northwestern University aims to design, synthesise and deploy new photocatalysts for activation and reduction of CO<sub>2</sub> using thermal catalysis and photocatalysis.

Tyndall's role in the project is to undertake first principles DFT simulations of new photocatalysts based on TiO<sub>2</sub> modified with nanoscale metal oxide clusters and evaluate the potential of these new compositions for visible light absorption, charge separation and the ability to activate CO<sub>2</sub>. This will involve large scale DFT simulations using DFT codes to develop new photocatalysts with visible light absorption, and study the fundamental reactions involved in CO<sub>2</sub> activation and reduction on these new materials. The most suitable materials designed in the simulations will be passed to the experimental partners for synthesis and characterization with feedback between experiment and simulation. Extensive travel between project partners will be required as will constant interaction with the partners.

Candidates with at least a 2.1 Bachelors degree (or equivalent) in Chemistry, Physics or Materials Science and, ideally, experience in modelling of metal oxides, are invited to apply for this position, which commences on September 1st 2014.

The successful candidate will be based at Tyndall and will enroll in the Chemistry department in University College Cork on a structured PhD program in which students undertake a range of technical and non-technical courses to enhance their general skills in addition to the research on their PhD topic.

Please apply in the first instances to [michael.nolan@tyndall.ie](mailto:michael.nolan@tyndall.ie) attaching a CV, motivation letter and a list of publications.

### **Responsibilities:**

- To undertake first principles simulations of TiO<sub>2</sub> surfaces modified with metal oxide nanoclusters
- To evaluate the effect of the modification on the energy gap of TiO<sub>2</sub>
- To study the interaction of CO<sub>2</sub> at these structures and understand factors that govern the activation and reduction of CO<sub>2</sub>

- To present the results of these studies to experimental partners and propose materials compositions for experimental study
- To attend and present project results and workpackage and project meetings
- To prepare and submit scientific publications
- To present at international conferences

**Requirements:**

- 2.1 Bachelors degree or higher (or equivalent) in Chemistry/Materials Science/ Physics.
- Experience in first principles simulations of metal oxides and reaction mechanisms desirable.
- A good understanding of solid state and materials chemistry is desirable