Postdoctoral Researcher – Design of Photocatalysts for CO_2 Activation

A 24 month researcher 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_2 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_2 using thermal catalysis and photocatalysis.

Tyndall's role in the project is to undertake first principles DFT simulations of new photocatalysts based on TiO_2 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_2. This will involve large scale DFT simulations using DFT codes with an emphasis on Car-Parinello type simulations to understand charge dynamics and fundamental reactions involved in CO_2 activation and reduction.

Candidates with an existing PhD and experience in modelling of metal oxides and reactions on oxides, are invited to apply for this position, which commences on September 1st 2014. Candidates with expertise in CP type simulations are particularly desired.

Please apply in the first instances to michael.nolan@tyndall.ie attaching a CV, motivation letter and a list of publications.

Responsibilities:

- To undertake first principles simulations of TiO_2 surfaces modified with metal oxide nanoclusters
- To evaluate the effect of the modification on the energy gap of TiO_2
- To perform calculations of charge localisation and charge dynamics in the new structures
- To study the interaction of CO_2 at these structures and understand factors that govern the activation and reduction of CO_2
- 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:

- PhD in Materials Science/Chemistry/Physics, **already graduated**, with deep experience in first principles simulations of metal oxides and reaction mechanisms.
- Experience using high performance computing systems and simulation codes
- Track record of publications and presentations in the pertinent areas
- Experience with Car-Parrinello simulations is desirable
- Track record of preparing and submitting scientific publications and presentations