

Postdoctoral Researcher - First Principles Simulation of Methanol Synthesis Catalysts

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 of catalyst development for methanol and higher alcohol synthesis. The BIOGO project, funded under the European Commission 7th Framework program, aims to develop new catalysts, with no precious metals, and that are poisoning resistant, for methanol synthesis from biogas and bio-oil. Tyndall's role in the project is to undertake first principles DFT simulations of new catalyst compositions and structures and identify suitable catalysts to be passed to experimental collaborators within BIOGO for synthesis and testing. The best catalysts will be scaled up to industrial production and applied in pilot scale reactors.

Candidates with an existing PhD and experience in modelling of metals and metal oxides and reactions on same, are invited to apply for this position, which commences on May 1st 2014. Please apply via <http://www.tyndall.ie/career/search>, selecting reference number MN-02 and following the instructions to complete the associated application form, attaching your CV and motivation letter.

Responsibilities:

- To undertake first principles simulations for methanol synthesis from syn gas on new metal oxide based catalysts
- To determine the most suitable catalyst structure and composition for passing to experimental partners within the project
- To study poisoning with sulfur containing species.
- To liaise closely with experimental collaborators within the project
- 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 in first principles simulations of metal oxides and reaction mechanisms.
- Track record of preparing and submitting scientific publications and presentations

Please apply via <http://www.tyndall.ie/career/search>, selecting reference number MN-2 and following the instructions to complete the associated application form, attaching your CV and motivation letter.