MONASH University
Engineering

Summer Research Program 2011/2012

Project Title Catalysts for synthetic fuel production – experiments and modeling

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Objective

Carry out experimental and modelling work to synthesise catalysts for production of synthetic fuel from coal and biomass

Description

Catalytic synthesis process has to deal with issues such as conversion of reactants and selectivity of the desired products. Even the best available catalyst today cannot completely eliminate undesirable by-products. Moreover, there is a significant drive to reduce fossil fuel dependence and to minimise carbon dioxide emission. Therefore, need for new and improved catalytic processes are more than ever.

Design and synthesis of catalyst has traditionally been based on trial and error basis. However, recent rapid progress in density functional theory (DFT) calculations for surface processes is the key development that has created the possibility of computer-based catalyst design. The current project will involve:

1. Computation design of new heterogeneous catalysts for syngas to dimethyl ether (DME) synthesis, using DFT.
2. Synthesis of several DME catalysts based on DFT calculations.
3. Characterisation of the prepared catalysts using XRD, NH_3-TPD and electron microscopy.
4. Evaluation of the DFT surface model based on the experimental findings.

This project has enormous practical significance.

The project will therefore suit a hardworking student with aptitude for both experimental and modelling work; some experience of using either Matlab or Comsol will be useful. The student will work alongside a PhD student and a Research Fellow.

We reserve the right to talk to the student prior to selection.