SEMS: RESEARCH PROJECT DESCRIPTION

1. Project Background and Description

Title: ***New routes to synthetic fuels: Vibrational strong coupling***

Description:

The production of chemicals commonly involves complex synthetic pathways in a sequence of site-selective reactions. However, the number of steps in the pathway is often increased by the presence of multiple reactive sites on the molecule. These additional sites may have a higher reactivity than the target site and lead to one or more side-reactions which decrease the reaction yield and pollute the product. For this reason, it is common to introduce protection and deprotection steps to prevent side reactions, or to follow more circuitous synthetic routes.

In this project we propose a new approach to site selective chemistry. By performing reactions in highly tuned cavities, we will modify the reactivity on the desired molecular sites. It will be possible to control the reaction simply by controlling the cavity dimensions to match the vibratrional energy of the targeted molecular bond.. In this way, reactions can be focussed on the desired sites, by-products eliminated and reaction rates controlled. Synthetic pathways will be shortened.

This proposal will focus on hydrogen production by water splitting and a key step in the production of synthetic fuel (methanol to dimethyl ether). We have deliberately built this proposal around reactions that are important for the manufacture of energy materials, since it is critically important that these materials are synthesised with minimal "built-in" energy. Companies operating in this area might be the first to benefit from the outputs of this project, but the understanding of reactor design for strongly-coupled reactions has benefits which extend to large parts of the industry.

2. Project Scope

Research project objectives:

1. *Develop reactors for chemical synthesis in the vibrational strong coupling regime.*
2. *Increase the rate of water splitting and decrease the voltage required through vibrational strong coupling.*
3. *Use vibrational strong coupling to facilitate a direct methanol to dimethyl ether reaction.*

3. Desired Skills from the Student

- Experience in any of:
  - Physical chemistry
  - Optical characterisation
  - FTIR
  - Chemical synthesis
  - Photolithography
- The ability to work in a laboratory environment.
- Qualifications in any of: Chemical Engineering, Materials Science, Physics, Synthetic Chemistry.

4. Supervisors

Primary supervisor: Dr Oliver Fenwick (School of Engineering and Materials Science)

Secondary supervisor: Dr Christian Nielsen (School of Biological and Chemical Sciences)