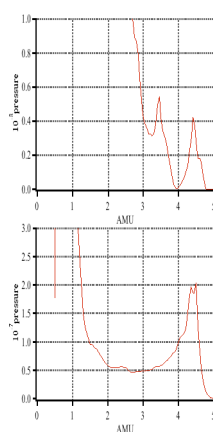


Projects in the John White group: contact jww@rsc.anu.edu.au

1. Photochemical water splitting

In this project the experiments aim to study the mechanism of the photoproduction using the deuterium isotope effect and maximize the production of Hydrogen from water using titanium oxide as the photocatalyst. The apparatus is already set up. We have produced mesoporous Titanium oxide thin films which do split water and I am keen to see what would happen if, instead of converting the amorphous titanium oxide to anatase at 380C as we have done in the past, we attempt conversion to rutile at 700C. The first thing to study is the stability of the mesoporous structure at high temperatures and whether carbon doping occurs at the elevated temperature. Optical spectroscopy will be used to study the TiO₂ band gap and x-ray diffraction the mesoporous structure. This will be a matter of empirical trials at different temperatures and the observance of the hydrogen production as a result of this treatment.

The mass spectra below show that even from 99.75% pure heavy water a lot of HD and H₂ is produced by the string isotope effect in the photochemistry. The references below are very recent papers (from a conference in Paris 2 July 2008) with a new view of the catalytic activity of TiO₂.



**Mass Spectrum
from irradiation**

**Mass Calibration
(with D₂)**



TiO₂ (011) reactivity **Science 317, 1052, 2007 Dulub et al.**

Oxygen terminated surface. Physical Review Letters 93, 036104, 2004

Enhanced photocatalytic activity - titanyl model. Another model JACS 129, 10427 (2007)

2. Lithium intercalation into Graphite

The Lithium -hydrogen- graphite interaction is central to the function of modern high capacity batteries The work that we did about 20 years ago on hydrogen adsorption by graphite intercalation compounds of potassium, rubidium and caesium showed how one could map the adsorption potential for the molecule by looking at the hindered molecular rotation and tunneling.

Recent references are: Hydrogen **induced nanostructures in graphite** Physical Review Letters 84, 4910, 2000, and Nature 380, 231-234, Hydrogen mirror.

The lithium - graphite compound is hard to make since lithium attacks glass and silica at a few hundred degrees centigrade - preferentially to carbon. The glass and silica then shatter as things cool because of the difference in coefficient of expansion. I thought of a way of making it about a year ago but we haven't tried it. It is to put the lithium into a sealed graphite crucible inside the glass or silica so that the only thing that the lithium vapour sees when heated is the graphite. I would like to try this if you are interested and then characterise the gas adsorption properties of the expected C₆Li compound.

We would have to use the VAC dry box at the Research School to manipulate the compound for diffraction, for example.

3. *Free protein - enzyme reactions*

We have recently found a way to prepare mono molecular films of protein at the air-water interface and to flush out the forming solution. This allows surface reactions between the isolated protein film and enzymes to be studied for the first time. A paper will appear in the journal "Soft matter" in about September 2008.

Within this category the immediate thing to try is whether enzymes which cut proteins can do the same thing to the surface adsorbed protein as they do in solution. I am particularly interested in the blood plasma proteins because I am hoping to do some work in the next three years on nanotoxicology where the protein-nanoparticle interaction is all important. This would be an exploratory project and its direction would be determined by what we find.