

## Crystal engineering published in *Nature*

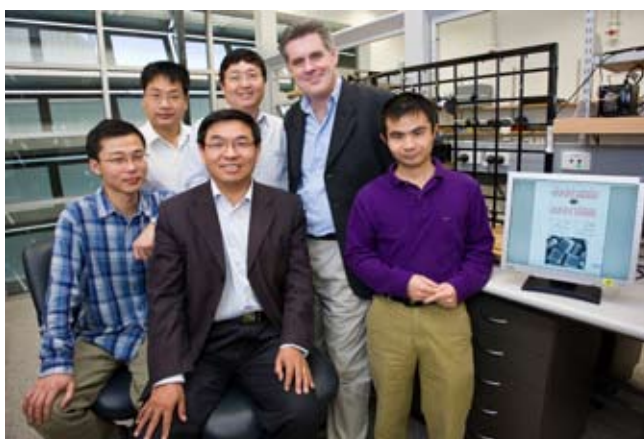
In a world-first, researchers from the ARC Centre of Excellence for Functional Nanomaterials (pictured below), in collaboration with the Chinese Academy of Sciences have combined theoretical computational studies and experimental techniques to synthesise a highly reactive and efficient photocatalyst. Owing to their scientific and technological importance as photocatalysts (among other applications), inorganic single crystals with highly reactive surfaces have long been studied. Unfortunately, surfaces with high reactivity usually diminish rapidly during the crystal growth process. A typical example is the photocatalyst titanium dioxide (anatase  $\text{TiO}_2$ ). Most available anatase  $\text{TiO}_2$  crystals are dominated by thermodynamically stable surfaces or facets (referred to as {101} surfaces in crystallography), rather than the much more reactive surfaces {001} – which account for only 3% of the total surface.

In a unique investigation combining theoretical and experimental techniques, the group have been able to effectively manipulate the crystal-growth process to create a morphology with a high proportion of reactive sites. Initial computational studies indicated that among the 12 non-metallic atoms investigated, controlling growth with fluorine (F) yields more stable atoms with a higher proportion of reactive surfaces.

Based on these theoretical predictions, the research group, led by Professor Max Lu, successfully engineered the surface and crystallographic characteristics of crystalline materials to synthesise uniform anatase  $\text{TiO}_2$  single crystals with a high percentage (47%) of reactive surfaces, using hydrofluoric acid as a morphology controlling agent. The fluorated surface of the single crystals can easily be cleaned using heat treatment to render a fluorine-free, high-purity anatase  $\text{TiO}_2$  surface without altering the crystal morphology.

This work illustrates the power of combining theoretical computational studies and experimental techniques to achieve engineering of surface and crystallographic characteristics of crystalline materials and has been recently published in *Nature* (H G Yang et al, *Nature*, 2008, 453, 638 (DOI:10.1038/nature06964)).

The well-defined, high-purity anatase single crystals synthesised in their work would be very useful as model crystals for fundamental studies of surface science. These crystals have promising applications in solar cells, photonic and optoelectronic devices, sensors and photocatalysis. ■



From left - Dr Gang Liu, Dr Huagui Sun, Professor Max Lu, Dr Shizhang Qiao, Professor Sean Smith, Dr Chenghua Sun

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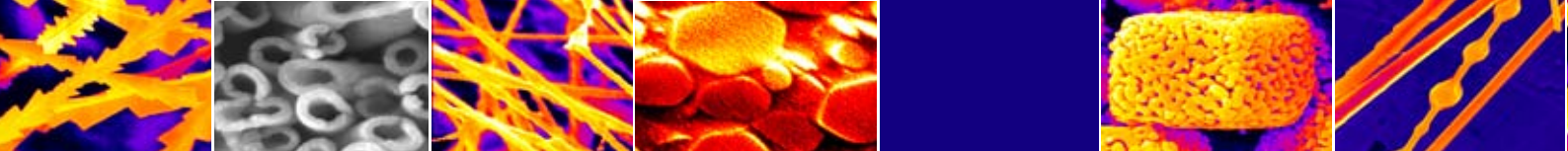
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## Project spotlight Vanadium nitrides for supercapacitors

Supercapacitors offer high capacitance in a small package and are able to release a large amount of energy very quickly. Their many other advantages are well-known (e.g. quick recharge), however there are some drawbacks which also need to be addressed.

A centre research project which brings together ANU PhD student Mr Alexy Glushenkov and University of Queensland researcher Dr Denisa Jurcakova investigates ways to overcome the high cost of current methods, increase performance and simplify manufacturing techniques.

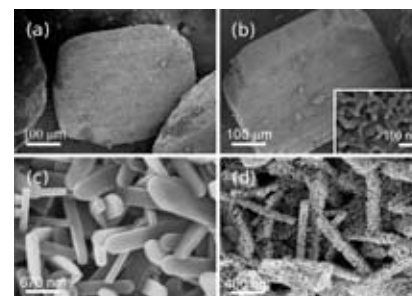
It is widely recognised that  $\text{RuO}_2$  provides the best pseudocapacitive properties, with energy densities up to 800 F/g. It is however very expensive. Recently, excellent pseudocapacitive behaviour has been reported for nanocrystalline vanadium nitrides (VN).

When 1M KOH aqueous solution is used as the electrolyte, these supercapacitors were able to provide reversible stable operation and deliver impressive capacitances.

In this project, Alexy and Denisa are using a  $\text{V}_2\text{O}_5$  ammonia reduction method as a means of producing VN materials for electrodes in supercapacitors. This approach is a simpler alternative to prepare nanocrystalline vanadium nitrides. It provides greater flexibility in fine tuning the structural details of the material such as external shape and size of porous particles and their internal morphology. The morphology of vanadium nitrides mimics that of initial  $\text{V}_2\text{O}_5$  precursors (see the SEM image, right). The advanced nanotechnology of vanadium oxide (nanotubes, scrolls, nanowires, nanorods and nanoparticles are reported, including ordered arrays attached to surfaces) can be used to produce analogous porous morphologies of VN by directly converting  $\text{V}_2\text{O}_5$  materials into vanadium nitrides.

As previous studies have only examined KOH as the electrolyte for VN

supercapacitors, this investigation is characterising its capacitive properties in other electrolytes. The performance of VN supercapacitors in acidic (1M  $\text{H}_2\text{SO}_4$ ), alkaline (1M KOH) and neutral (3M NaCl, 3M KCl) aqueous solutions was compared. Additional characterisation methods such as XRD, TEM and XPS were employed to explain the mechanism of capacitive properties and cycling characteristics of vanadium nitrides. ■



SEM images of initial  $\text{V}_2\text{O}_5$  materials (a, c) and obtained VN materials (b, d). The inset in (b) shows the porous nature of the particle.

## Upcoming Events

### 17th International Conference on Photochemical Conversion and Storage of Solar Energy



The development and sustainable management of natural resources for energy and environmental purposes continues to grow in both relevance and

importance, with solar-based technologies playing a significant role in addressing these issues. The biennial International Conference on Photochemical Conversion and Storage of Solar Energy (IPS) series provide an excellent forum for academic and industry personnel to gather and exchange knowledge and ideas in

related fields.

The 17th International Conference on Photochemical Conversion and Storage of Solar Energy is to be hosted for the first time in Sydney, Australia, from the 27th July to 1st August, 2008 and will be held at the Sydney Convention and Exhibition Centre, located in the picturesque Darling Harbour. The ARC Centre of Excellence for Functional Nanomaterials, Centre of Excellence for Photovoltaics and Centre of Excellence for Electromaterials have united in an effort to maintain the high quality delivered by previous IPS events.

Confirmed speakers, program information, travel details and registration information can be found at the conference website at

[www.ips17.com](http://www.ips17.com) ■

### ARCCFN Conference 2008 Advancing Functional Materials

This year's centre annual conference will be held on the Gold Coast (QLD), from the 5-7 November 2008.

The annual conferences, 'Advances in Functional Nanomaterials' enable centre participants from all the nodes to meet and discuss their research. Representatives from industry are also invited to attend and participate in the conference.

Check the Centre's website for regular updates. ■



## Communication news

### ARCCFN new website launched

The new ARCCFN website was launched in June ([www.arccfn.org.au](http://www.arccfn.org.au)). The website includes comprehensive information on projects, upcoming events, centre news and highlights. The latest and past editions of Nanomatters are also available online, and you can also register to have future editions emailed or posted to you.

### Nature Paper

Centre research published this month in *Nature* attracted a lot of media attention, with articles in *The Courier Mail*, *The Australian*, *The Age* and *The Sydney Morning Herald*. ABC radio also broadcast the story across Australia. Given the small print space devoted to science reporting, it was great recognition of the relevance and significance of the Centre's achievements.

### Lightanate project on youtube

A new photocatalyst *Lightanate* developed by Centre researcher Dr Lianzhou Wang and colleagues featured on a 6:00pm news bulletin on Brisbane's Channel 7. The feature, entitled 'New Fuel' reported on *Lightanate*'s potential to fast-track a transition to hydrogen fuel. The report, which included short spots with Professor Max Lu and Dr Wang, while brief, was an excellent achievement and gave the centre exposure to a vast, general audience. The full report can be viewed on youtube at the following link

[http://www.youtube.com/watch?v=HKH\\_iKkTnPE](http://www.youtube.com/watch?v=HKH_iKkTnPE)

## Federation Fellowships



Professor Aibing Yu

Congratulations to Professors Aibing Yu (Centre Chief Investigator and project leader UNSW) and Max Lu (Centre Director) who were awarded Federation Fellowships; Professor Lu for the second time. The prestigious Australian Research Council Federation Fellowships are considered to be the premier scientific appointment in the country and are aimed at attracting and retaining world-class researchers. The scheme supports and encourages researchers of international renown to conduct research of significant national economic, environmental, cultural and social benefit. It is a great achievement that two of only 14 federation fellows announced in 2008 are part of the Centre. ■

## 2020 Summit

In recognition of his contribution to science and excellence in research, centre director Professor Lu was selected to attend the 2020 summit in Canberra to participate in the *Future Directions for the Australia Economy* session. In a double honour, Professor Lu carried the Olympic torch in Canberra during the Australian leg of the relay in April. ■



Astute manager Dr Fouad Haghseresht and Centre director Professor Max Lu

Astute Nanotechnology's first birthday celebration was a success, with over 80 people attending, 50 of those from industry. Many of the industry representatives were fresh faces, new to the centres research capabilities. During the evening, guests were able to tour the laboratory facilities and listen to presentations from various researchers, who presented work of direct relevance to the industry guests. There was also ample opportunity for researchers and guests to network and ask questions.

Dr Haghseresht has recently returned from Boston where he attended NSTI (Nano Science and Technology Institute) Nano conference, *tech connect* event. Nanotech 2008 is the largest and most comprehensive technical and business event in nanotechnology world-wide with over 30 technical and business symposia. These annual conferences bring together scientists, IP managers and venture capitalists. Dr Haghseresht gave three presentations and formed some valuable links with US Venture capitalists. ■





ARC Centre of Excellence for  
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## International activities and awards

**Mr Akshat Tanksale and Ms Siswati Lestari** (PhD students) have both been awarded the Young Scientist Award by the Council of the International Association of Catalysis Societies. Candidates were selected on the basis of their extended abstracts and they will receive their awards (which covers all travel costs) at the conference in Seoul, Korea in July. ■



**Dr Denisa Jurcakova**, post-doctoral research fellow, has been awarded the Brian Kelly award for 2008 by the International Carbon Society. The prize of £500 will be presented at Carbon 2008 in Japan this July. Only one Brian Kelly prize is awarded each year world wide, and is recognition of Dr Jurcakova's contribution to carbon research. ■

**Dr Bradley Ladewig**, post-doctoral research fellow, has been awarded the Australian Institute of Energy - Energy Council of Australia 2008 Study Scholarship. Valued at \$6,000, the scholarship will support Dr Ladewig's attendance at the International Congress on Membranes and Membrane Processes in Hawaii in July, where he has been invited to present his work. The scholarship will also allow Dr Ladewig to attend a one week course on neutron scattering at ANSTO's Neutron School on Materials, where he was successful in obtaining one of only 30 available places. ■



**Mr Anthony Musumeci**, PhD student on the nanotoxicology project, will spend three months working with Dr Tihana Rajh from the Center for Nanoscale Materials, Argonne National Laboratories in Chicago (USA). Dr Rajh is in an important strategic collaboration in the larger project that aims to assess the biological interactions and toxicity of a range of different industrially relevant nanoparticles. Anthony will spend three months in Dr Rajh's laboratories synthesising tailored libraries of TiO<sub>2</sub> nanoparticles and developing fluorescent and radiolabeling methods to enable better

toxicological assessments. He will also present some work at the World Biomaterials Congress in Amsterdam, and attend the conference Nanotox2008 in Zurich, Switzerland. This research visit and conference travel is supported by a UQ Graduate School Research Travel Grant (\$5000), ARCNN overseas travel fellowship (\$5000) and AINSE International Conference Travel Scholarship (\$900). ■

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