The Mission and Objectives of the Nanochemistry Research Institute

Mission

“To conduct world class research and development, commercialisation and research training in nanochemistry”

Objectives

The Institute aims to:

• Concentrate research activity in areas of competitive advantage to meet identified industry needs and opportunities
• Produce high quality research graduates who are sought after by industry
• Build sustainable, world class and multidisciplinary research capacity
• Have a tangible positive impact on the community with respect to sustainable social, health, economic and environmental development
Chief Scientist Visits the NRI
Commonwealth Chief Scientist Dr Robin Batterham visited the Department of Applied Chemistry to tour facilities in the Nanochemistry Research Institute. Dr Batterham was accompanied by Dr Joseph Patroni of the State Government’s Office of Science and Industry, as staff of the NRI showed the visitors some of the Institute’s world-class facilities in Computational Chemistry and Scanning Probe Microscopy.
Dr Batterham was shown examples of NRI Projects demonstrating the strength of nanochemistry as a bridging activity between the traditional physical sciences of nanotechnology and the life sciences of biotechnology.

Premier’s Research Fellowship to Professor Gale
Professor Julian Gale was presented with an inaugural Premier’s Research Fellowship worth $1 million over four years. Professor Gale will use computer simulation to model the behaviour of atoms in molecules and solids to improve understanding of how they work.

Grant Successes
Professor Gordon Parkinson and Professor Kate Wright, in conjunction with A/Prof Craig Buckley, Department of Applied Physics, and A/Prof Tim St Pierre, University of Western Australia, were awarded an Australian Research Council - Discovery Project grant for the project entitled “Ferrihydrite: Fundamentals of a Natural Nanomaterial”.
A/Prof Mark Ogden, in conjunction with Dr Heather Benson and Dr Yan Chen, Department of Pharmacy, Dr Neil Rothnie, Monash University, Dr Peter Taylor and Dr Steve Wilkinson, Chemistry Centre, were awarded an Australian Research Council - Linkage Project grant for the project entitled “Micro- and nano-particulate delivery systems for chemical and biological weapons: physical characterisation and risk assessment”

Small Science - Big Opportunity
The Nanochemistry Research Institute hosted a visit by representatives from Frontier Carbon Corporation (Japan) and its parent company, Mitsubishi Corporation (Japan), who presented new research into nanocarbon technologies.

Teaching Awards
Dr Mauro Mocerino received the Premier’s Prize for Excellence in Science Teaching 2003. A/Prof Mark Ogden was presented with the Curtin University Excellence in Teaching Award in 2003.

AJ Parker CRC for Hydrometallurgy
AJ Parker CRC for Hydrometallurgy and Curtin through the NRI signed a Memorandum of Understanding in September 2003.
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Welcome to the second Annual Report of the Nanochemistry Research Institute (NRI). The NRI was formally established as a Research Institute in December, 2001, and this establishment is a recognition by Curtin of the high quality and level of activity in nanochemistry within the University. I am extremely grateful to all the staff and students within the NRI and elsewhere within Curtin, our industrial partners, and national and international collaborators, whose continued dedication and support have made possible the achievements and level of international standing attained by the NRI.

People are the most important part of NRI, and we are delighted to welcome Mrs Elisabeth Grant as our Projects Coordinator, Professor Julian Gale from Imperial College London as the inaugural Western Australian Premier’s Fellow in Computational Chemistry, Professor Kate Wright from University College London and A/Prof Alistair Fletcher from CSIRO. Many congratulations also to Dr Mauro Mocerino for winning the Premier’s Prize for Excellence in Science Teaching and A/Prof Mark Ogden for his award of the Curtin University Excellence in Teaching Award.

When we first established NRI it was quite common to hear the question “What is Nanochemistry?”, but already it has become a much more widely recognised term. Briefly, nanochemistry is a discipline that is concerned with understanding and using the unique chemical properties that belong to assemblies of atoms and molecules which have approximate sizes in the range of 1 to 100 nanometres. Examples of objects of this size include the exciting new form of carbon, fullerenes and carbon nanotubes (the diameter of C_{60} is 1nm), and viruses (typically tens of nm in size). These examples illustrate another important aspect of nanochemistry: namely, that it forms a bridge between the physical sciences and engineering of conventional nanotechnology and the biology of the life sciences.

The Annual Report contains examples of some of the nanochemistry research activities being carried out within the NRI. These activities are founded on our core strengths of scanning probe microscopy, computational chemistry and synthesis of organic molecules that form supramolecular systems. In parallel with a focus on strategic fundamental research, our activities are directed towards applications in the resource (mineral, oil and gas) and agricultural / biomedical sectors. As well as having a very strong postgraduate training and research activity, staff of the NRI play a leading role in the delivery of undergraduate teaching through the BSc degree in Nanotechnology, in collaboration with the Department of Applied Physics.

At an organizational level, as well as consolidating the existing infrastructure of the NRI, much effort has been applied this year in strengthening our links with Edith Cowan University, Murdoch University and the University of Western Australia on two major fronts. First, we have prepared and submitted a strong case for the establishment of a Centre of Excellence in Nanochemistry within Western Australia including the NRI at Curtin University, the School of Biomedical and Chemical Sciences and the Department of Physics at the University of Western Australia, and the Murdoch University Surface Analysis Laboratory. Secondly, NRI is a core partner in the proposal to the State government to form Western Australia’s Electron Science Valley under the Western Australian Major Research Facility Program. On a national level, the NRI continues to make major inputs to the AJ Parker Cooperative Research Centre (CRC), and is part of the Australian Biosecurity CRC and the Sustainable Resource Processing CRC, the latter two of which commenced activity in 2003.

This is an exciting time globally, with much activity in nanotechnology; by focusing on the niche area of nanochemistry, the NRI is able to secure a strong position internationally, and help bring the coming benefits of the nanotechnology revolution to industry and the wider community of Australia.

Professor Gordon Parkinson
Director of the Nanochemistry Research Institute
Organisational Structure

The NRI Structure

The management structure of the NRI consists of a Board, Director, Projects Co-ordinator and Project Area Leaders. The Director answers to the Board, with the Projects Co-ordinator and Project Area Leaders answering to the Director. A Scientific Advisory Committee will give scientific and commercial feedback to the Board and the Director.

The Director oversees all projects and provides technical input when necessary, as well as managing the strategic direction of the Institute. The Projects Co-ordinator ensures all administrative details for projects are completed as well as providing information to the Director on the financial, resource and staff management issues within the Institute. The Project Areas within the Institute are led by Associate Professor Mark Ogden and Dr Mauro Mocerino (Supamolecular and Synthetic Chemistry), Associate Professor Andrew Rohl and Professor Julian Gale (Molecular Modelling), Dr Manijeh Reyhani (Scanning Probe Microscopy) and Dr Eddy Poinern (Carbon Technologies).

The Board will consist of approximately 6 members. It is proposed that two members will be from Industry, one will be the Deputy Vice Chancellor – Research and Development, one will be the Executive Dean of the Division of Engineering and Science and a fifth member will be from an outside university. The Director will be the Executive Officer.

Board of Management

Board of Management has not yet been appointed due to the development of a business plan and application for the Western Australian Nanochemistry Research Institute (WANRI) through the WA State Government Centre of Excellence Program, which was submitted at the end of the year. The Board of WANRI will be commensurate with the Board of the NRI. However, since the Institute is a multi-institutional, State based institute, other considerations need to be included in the final composition of the Board.

Staff

The researchers within the Nanochemistry Research Institute bring together complementary skills and expertise from a variety of fields of research. This unique combination allows research conducted in one discipline to be applied in another, leads to synergy and innovation, and in conjunction with the national and international collaborations already established, there is potential to expand and develop research outcomes for an even greater variety of disciplines, nationally as well as internationally.
Researchers

Professor Gordon Parkinson
BSc(Hons), PhD, FRSC, C.Chem, FRACI

Crystallization, in particular elucidating crystal growth mechanisms; scanning probe and electron microscopy; innovation.

Professor Julian Gale
BSc(Hons), PhD

Development and application of computational methods for nanotechnology and materials science.

Associate Professor Andrew Rohl
BSc(Hons), D.Phil

Computer molecular modelling of crystal growth inhibitors and simulation of crystal growth processes

Associate Professor Mark Ogden
BSc(Hons), PhD

Control of crystal growth, particularly interactions of additive or impurity molecules; and tailor making additives; macrocyclic chemistry

Dr Mauro Mocerino
BSc(Hons), DipEd, PhD

Synthetic organic chemistry and macrocyclic chemistry, particularly calixarines; and chemical education
Researchers

Dr Tuna Dincer  
BSc, PhD  
Lactose crystallization and food science

Dr Sean Fleming  
BSc(Hons), PhD  
Computational Chemistry and programming

Professor Leslie Glasser  
BSc(Hons), PhD, FRSC, C.Chem  
Electrical and dielectric properties of insulators; properties of hydrogen bonded liquids; thermal processes in solids; computational molecular modelling of solids

Dr Franca Jones  
BSc(Hons), PhD  
Nanochemistry and crystal engineering; precipitation of solids from liquids; interfacial chemistry; adsorption chemistry

Dr Eddy Poinern  
BSc(Hons), PhD  
Carbon and fullerene technology; and scanning tunnelling and atomic force microscopy
Researchers

**Dr Manijeh Reyhani**
BSc (Materials Engineering), MSc, PhD

Crystallization, in nanoscale and real time; scanning probe and electron microscopy

**Dr Bill Richmond**
BSc(Hons), PhD

Nanoparticle synthesis and characterisation of metal oxides and silicates

**Dr Andrew Stanley**
BSc(Hons), PhD

Interfacial chemistry, chemical speciation, aqueous crystallization and photoelectrochemical energy conversion (left in July 2003)

**Dr Stefano Piana**
SSc(Hons), PhD

Classical and *ab initio* molecular dynamics simulations of solids, surfaces and biological macromolecules

**Associate Professor Alistair Fletcher**
BSc(Hons), PhD

Properties and applications of fullerenes and carbon nanotubes; Atomic force microscopy and applications in mining and energy systems; Commercial application of nanotechnology through entrepreneurship, including construction of a Master’s course in Entrepreneurship and Technology
Research Assistants

Mr Peter Chapman
BSc (App. Chem)

Mr Chapman assists in the Scanning Probe Microscopy Facility, maintaining equipment and performing experiments.

Mr Allan Oliveira
BSc(Hons)

Mr Oliveira works in the organic synthesis laboratory and on the “Optimisation of Crystal Growth” project. Mr Oliveira synthesises the majority of additive molecules used within the NRI.

Mr Tristan Upson
BSc(Hons)

Mr Upson was involved in the “Control of Scale Formation” and TiWest projects within the NRI. Mr Upson left the NRI in August to take up a position at Nabalco.

Directorate Staff

Mrs Elisabeth Balchen Grant

Mrs Grant is the Projects Co-ordinator for the NRI and deals with all administrative and financial matters involving industry funded projects, grants awarded and NRI matters. Mrs Grant is the point of contact for the NRI.

Ms Claire Hitchen

Ms Hitchen is the Personal Assistant to Professor Gordon Parkinson and prepares Prof Parkinson’s diary, organises all meetings and prepares all travel document requirements for the NRI.
Research Overview

Research in nanochemistry demands a multidisciplinary approach. Projects can involve bulk synthetic chemistry, computational molecular modelling, advanced microscopy techniques, even the synthesis of new molecules designed to spontaneously assemble into complex architectures. This is reflected in the Institute’s three core areas of expertise.

- The molecular simulation/computational chemistry/molecular modelling research group is one of the strongest in Australia, and is recognised worldwide. A solid theoretical basis is used to understand and visualise what is occurring at the nano scale. Members have ongoing involvement in the development of several simulation software codes that are in demand around the world; and have significant computing hardware.

- Nanocharacterisation expertise, encompassing a world class scanning probe microscopy facility, microscopy and analytical facilities, enables the real-time observation of nanoparticulate growth processes.

- Expertise in nanoreactions extends to the use of nano-containers, for molecular recognition, chemical storage, or to direct reactions on an extremely small scale. Capabilities in supramolecular and synthetic chemistry ensure that target compounds can be tailored to a specific size, shape and functionality, for particular applications, such as additives for crystal growth modification, scale mitigation, or product improvement.

Research Outcomes
Scanning Probe Microscopy

BACKGROUND
The Scanning Probe Microscopy Facility is managed by Dr Manijeh Reyhani. The Facility consists of instruments that provide very high resolution, three dimensional surface topography on an increasing variety of samples and are powerful tools for surface examination. The instrumentation has been built up over the life of the NRI and is now considered to be a world-class facility for research and development.

ATOMIC FORCE MICROSCOPE (AFM)
The Atomic Force Microscope (AFM) uses the sense of touch, and measures topography by mechanically moving a sharp probe across the samples to “feel” the contours of the surface in a manner similar to a phonograph stylus tracing the grooves of a record. Moreover, it can operate under liquids, including the corrosive solutions frequently encountered in industry.

Capabilities of AFM
- Atomic resolution
- *In situ* liquid cell under ambient conditions
- Phase imaging, for the study of composite materials, magnetic alloys, etc.
- Large sample imaging capability
- *In situ* imaging of samples in corrosive fluids (high and low pH) and at high temperatures (up to ca 100°C)
- Operation in contact and intermittent contact modes
- Sample imaging in controlled gaseous environment (for air sensitive samples, etc), with glove box for transfer.
- Contact mode and “tapping mode” operation (for viewing soft samples and weakly adsorbed species)
- MAC Mode (Highest resolution intermittent contact technique in liquid)
- Measurement of interparticle forces

SCANNING TUNNELLING MICROSCOPE (STM)
It is now possible to probe different metallic and semiconductor surfaces at high resolution. Atomic and molecular resolutions on surfaces are routinely achievable with the STM. In addition, the technique can operate in various environments such as UHV, liquids and at different temperatures. The inventors of STM, G. Binnig and H. Rohrer received part of the 1986 Physics Nobel prize in recognition of the contributions of STM to science.

Capabilities of STM
- Surface study of metallic thin films
- Investigation of ion selective electrode surfaces
- High resolution study of graphite and adsorbates
- Gold on Mica studies

*In situ* STM images of graphite made under a solution of KAu(CN)$_2$/KOH/ CaCl$_2$
Supramolecular and Synthetic Chemistry

The Research Area of Supramolecular and Synthetic Chemistry is headed jointly by Dr Mauro Mocerino and A/Prof Mark Ogden, with Allan Oliveira as their Research Assistant.

Supramolecular chemistry is often described as “chemistry beyond the molecule”. That is, we are interested in controlling intermolecular interactions; with appropriate design of the molecular components, such interactions can drive the spontaneous assembly of nanoscale structures which are much too large to be accessed via traditional synthetic chemistry.

The aim of this program is two-fold. One is to probe the origins of selectivity in intermolecular interactions, ranging from interactions between a metal cation and a synthetic receptor, to those between an enzyme mimetic and its biological target. The other is to provide the expertise and capabilities to synthesise target molecules, required in this program, and many other activities within the NRI. The bulk of this research is performed by graduate students of the NRI, and these projects are described in the following pages.

A specific area of expertise is the chemistry of the macrocycles known as calixarenes. These “basket-shaped” molecules are readily synthesised on a large scale, and can be chemically modified in many different ways. The resulting products are being used as crystal growth modifiers, components in nanoscale assemblies and crystal engineering, and as receptors for metal ions in ion selective electrodes. The group also has experience with other common supramolecular building blocks, such as crown ethers, dendrimers and so on.

A subset of the calixarene focus is the preparation of a variety of chiral calixarenes. There are two principal methods employed in our investigations, (i) Lewis-acid catalysed condensation of asymmetric resorcinol units and aldehydes to give C4 symmetric calix[4]resorcinarenes and (ii) introduction of chiral amino acid moieties onto the calixarene framework through amide linkages or via a Mannich type condensation. The use of these chiral calixarenes is being investigated in crystal growth modification, chiral recognition and catalysis.

Collaborative links with WABRI (Western Australian Biomedical Research Institute) have resulted in the recent increase in organic synthesis activities in this program. The overall project aim is to develop an effective insulin mimetic for oral administration that will stimulate the insulin receptor to lower blood glucose and give better glycaemic control for diabetics. An orally administered non-protein based drug has the advantages that it is a less expensive therapy, it alleviates the discomfort, inconvenience and risks associated with injections, would be cheaper to produce and would have better shelf-life, storage and distribution properties. Recent research at WABRI has identified a compound (IM140) that could be further developed into a suitable insulin mimetic. The aim of this research project is the synthesis of IM140 analogues and to test their activity in a range of bioassays.

The program has national and international collaborative links with groups including Dr Cameron Kepert (Crystal engineering, Uni. Sydney), Dr Phil Gale (Anion receptors, Southampton, UK), Prof. Allan White (structural chemistry, UWA) and Prof. Harry Heaney (chiral resorcinarenes, Loughborough, UK).
The Research Area of Computational Chemistry at the Institute is headed jointly by A/Prof Andrew Rohl and Prof Julian Gale. Prof Gale joined the Nanochemistry Research Institute as one of only two Premier’s Research Fellows in Western Australia. This research area is a world-leading facility that is involved in developing state-of-the-art simulation packages, both computational engines and graphical display programs. It is extremely well equipped for large-scale computations of solution, bulk and surface structure, energetics and physical properties.

Computational methods possess the capability to provide detailed understanding of chemical and physical processes at the atomic, or even electronic, level. This makes them an essential tool in the fields of chemistry, physics, materials science, mineralogy and many other disciplines through the ability to predict structure-property relationships. Simulation methods can be utilised for the modelling of solids, surfaces, polymers, liquids, as well as the gas phase.

**SIMULATION OF BAYER LIQUORS**
Molecular dynamics has been used to probe the structure of concentrated basic aluminate solutions. The simulations showed that ion pairing between sodium and aluminate is ubiquitous and this allows aluminates to approach each other and react to form larger assemblies.

**SURFACE STRUCTURES**
We have built an impressive array of surface simulation tools within the Laboratory. We have used these tools to simulate the surface reconstruction of calcite for the first time.

**NANOTECHNOLOGY**
A range of simulations are being performed to investigate the unique properties associated with materials when their dimensions are of the order of a nanometre. Projects include the storage of hydrogen within carbon nanotubes and the study of arrays of quantum dots.

![Theoretical AFM image of the (001) face of barite, calculated by rolling a probe atom over the surface.](image1)

![A crystal growth inhibiting molecule docked into a step of a calcite surface](image2)
The NRI conducts many projects ranging from applied to fundamental research, industry contracts to grant projects, and projects that fall within the auspices of the Parker Centre.

**Parker Centre Projects**

The NRI is the primary vehicle through which Curtin University carries out research and delivers outcomes to the AJ Parker CRC for Hydrometallurgy (Parker Centre). Any project that is hydrometallurgical in nature is classed as a Parker Centre project and all reporting responsibilities associated with Parker Centre projects are met. The following projects range from confidential industry funded work to fundamental research funded by the Commonwealth and State Governments, and are conducted as Parker Centre projects.

**P625 – Incorporation of Impurities in Gibbsite in the Bayer Process**

The AMIRA Project P625 “Incorporation of Soda into Gibbsite in the Bayer Process” is a collaborative project with CSIRO Minerals and several Australian alumina companies and involves members of the Alumina Program and Crystallization Program of the Parker Centre. The project commenced in July 2000 and was completed in June 2003. This project is Commercial in Confidence.

**Optimisation of Causticisation in Bayer Liquors through Crystallization Chemistry**

This project originally started in November 1998 and was a three year project sponsored by Alcoa World Alumina. The project was extended for a further 12 months in 2002. The techniques employed in this project covered crystallization fundamentals, wet chemistry techniques as well as the integration of computational molecular modelling results into the experimental program. Both projects are Commercial in Confidence.

**Investigation into Reducing Scaling in the Process and Effluent Streams at TiWest**

Scale in industrial processes is an on-going problem, and the Crystallization Program of the Parker Centre is conducting research into this area at a fundamental level as well as for industry clients, as part of the Parker Centre. This project commenced in April 2002 and should be complete in the first half of 2004. This project is Commercial in Confidence.

Other major ongoing Parker Centre projects includes:

- Optimisation of Crystal Growth
- Fundamentals of Scale Formation
- Fundamentals of the Fate of Silica and Iron Impurities in Hydrometallurgical Operations

Crystallizers at an Alumina Refinery
Optimisation of Crystal Growth

INTRODUCTION
This project focuses on the fundamental processes that underlie and ultimately control the production of crystals in an industrial plant. The precise factors governing properties such as the external shape or morphology of a crystal, the polymorph (crystalline form) produced and the rate of growth are being investigated. Carefully chosen model systems are being used to study particular phenomena, facilitating the fundamental studies. The knowledge obtained is being applied to industrial systems.

ACTIVITIES
Studies of calcite crystal growth using *in situ* atomic force microscopy continue to be a significant focus. The technique has been successfully extended to observe crystal growth at atomic resolution. Comparison of atomic resolution images in the control system with those obtained in the presence of additives suggests that significant surface restructuring is taking place. It is not yet clear whether the differences observed are due to coating by the additive, or a change in the calcite surface structure, and work is continuing to clarify this. In particular, molecular modelling studies are being used to provide a direct link to the atomically resolved images. Larger additive molecules with well-defined structures are also being studied in an effort to visualise individual additive molecules on the crystal surface. Correlation of additive structure (incorporation of carboxylate and phosphonate groups in particular) with efficacy of crystal growth modification has been achieved.

The introduction of the MacMode technique for surface characterisation and crystal growth monitoring has assisted this work. Mac Mode is an oscillating cantilever method of imaging, which uses a magnetic field as the cantilever driving mechanism with the Molecular Imaging Instrument. Like other AC techniques, the cantilever is driven at high frequencies and the surface is monitored by changes in the amplitude. Monitoring is much slower than conventional AFM imaging, therefore stability of the solution in real time becomes a limitation. However, the advantages of the technique are better resolution and no disturbance of the surface. Images produced by this technique are shown below.
Investigation of the growth of potash alum (KA1(SO4)2.12H2O) crystals in aqueous solution using electron microscopy and in situ AFM has started. Experimental work shows that the growth of crystals on the (111) face occurs by step movement; addition of gallic acid causes roughening of the steps and inhibits the growth. The high solubility and fast step movement makes this a challenging system to work with, but high resolution imaging has been achieved.

*Studies on the formation of the fine crystals of Barite:*
Formation of fine barium sulphate crystals was examined by contact AFM. The following particles are the crystals formed in control solution without the addition of any additives. The presence of a growth spiral can be observed on the surface. This is the first time growth spirals have been observed on a barite crystal grown *in situ.*

*Studies on the cleaved crystal surfaces of Barite:*
Nucleation on the cleaved Barite surface is observed after solution is added. In a highly supersaturated solution nuclei are formed on the surface, and the growth of these nuclei is monitored, as shown in the image series.
In situ investigation of the growth of Calcium Oxalate using AFM.
Calcium Oxalate is a system of importance to industry, and in biological systems (kidney stones). The images show the typical morphology of the calcium oxalate crystals formed. AFM studies are being carried out to investigate the fundamental mechanisms of growth in these crystals.

Very limited information is available on *in situ* AFM of these crystals and so these studies have the potential to offer new insight into the growth of calcium oxalate crystals. Crystals formed so far are large and rough for AFM, but show the typical structure. These images are an AFM image of calcium oxalate in equilibrium solution.

![Calcium Oxalate Crystals](image)

**FUTURE WORK**
The detailed information about additive–crystal surface interactions gained in the course of this project is the first step to improved understanding of crystal growth processes and additive design. The project will now focus on correlation of results between the various crystal systems under investigation, and further development of additive structure–efficacy relationships.

**OUTCOMES**
- Crystal growth studied at *nanoscale and in situ*.  
- Links between additive structure and growth inhibition clarified.  
- Skills in the use of new techniques to investigate nanoscale surface characterisation developed.
OBJECTIVES
To gain a fundamental understanding of the chemistry and hydrodynamics of supersaturated solutions that hinder the formation of crystalline scale deposits.

Both engineering and chemical strategies are being investigated in order to devise mitigation strategies to a serious industry-wide problem. A theoretical understanding of how existing empirical scale prevention strategies work must first be obtained. To this end, a combined approach of micro and macroscopic experiments and molecular modelling is being used to determine effective control strategies, based on fundamental models of microscopic phenomena.

ACTIVITIES
The model system of barium sulfate has been used to test the effectiveness of various inhibitors. A paper on the role of calcium on the inhibitory efficacy of additives on barium sulfate inhibition has been published. The effect of calcium alone increases the solubility due to an increase in ionic strength; however, calcium ions also incorporate into the lattice and possibly even poison surface growth features. At high calcium levels, calcium ions lower the effective supersaturation due to ion-pair formation of calcium with sulfate. When additives are present another mechanism also comes into play, whereby the calcium cations promote the precipitation of barium sulfate. This paper has been submitted and we await a response. The calcium cations are not always complexed to the organic additive; thus, it is believed that a simple concentration gradient exists around the organic species which promotes the precipitation of barium sulfate either through electrostatic interactions (the sulfate to calcium interaction) or by lowering the critical nucleus size required for precipitation to occur.

Work is ongoing in obtaining Fourier-transform infrared (FTIR) spectra of the adsorbed additives (carboxylates) on barium sulfate. This work is focusing on obtaining adsorption isotherm data for carboxylate additives by FTIR. The technique being used is a surface technique called DRIFT (Diffuse reflectance). Data on NTA (nitrilotriacetic acid), showed a small adsorption plateau suggesting that NTA adsorbs only onto specific features of the surface (eg. kinks). Currently, data are being obtained for EDTP (ethylenediamine tetraphosphonic acid). The phosphonate additives have infrared bands in the same region as the sulfate bands; thus, a different analytical technique is currently being assessed to obtain adsorption isotherms for these additives.

Potassium perchlorate (a system chosen because it is isostuctural with barium sulfate, but has a much higher solubility) was found to be an interesting system whereby several additives tested appeared to inhibit precipitation to the same degree, despite the fact that the additives contained different functional groups. The
additives had a similar structural backbone suggesting that lattice matching was the dominant mode of interaction for these additives. However, these same additives on barium sulfate suggested that charge matching was important. Thus, solubility appears to play a role in the efficacy and mode of interaction for various additives. This will be investigated further.

AFM work on barium sulfate has commenced using natural, cleaved samples. This allows us to compare with literature already published as well as investigating new areas. Study of the effect of additives on the growth of barium sulfate is currently underway and we have successfully imaged the (001) barium sulfate surface with NTMP (nitrilotrimethylene phosphonic acid) at atomic resolution. Molecular modeling is being conducted to interpret the AFM images.

**FUTURE WORK**
- The effect of temperature on inhibitors.
- Further spectroscopic investigations and adsorption isotherm data on additives obtained.
- Further AFM work to determine the mode of inhibitor interaction at the atomic level.
- Molecular modelling will expand to stepped and defect surfaces.

**OUTCOMES**
- Calcium promotes nucleation in the presence of additives
- Adsorption of NTMP is at specific surface features
- Solubility affects the mode of interaction of inhibitors

Top and side view of the NTMP molecule adsorbed on the barium sulfate (001) surface – the most energetically favourable configuration as determined from molecular modeling.
Fundamentals of the Fate of Silica and Iron Impurities in Hydrometallurgical Operations

OBJECTIVES
This project is one of the core projects of the AJ Parker CRC’s Crystallization Program, and its general objective is to build on existing areas of strength within the Crystallization team in order to develop a strong research group with a knowledge base and expertise in the study of iron and silica precipitation. In more specific terms, the project has the following three aims:

- To develop fundamental understanding of hydrolysis reactions involving iron and silicate species.
- To develop fundamental understanding of the mechanisms of action of scale inhibitors and other additives used for control of iron/silica precipitation.
- To recommend strategies for control of iron/silica precipitation in specific processes.

ACTIVITIES
We have found that the transformation of ferrihydrite to more crystalline phases such as goethite and hematite can be promoted by the addition of ZnS to the reaction mixture. This discovery may have important implications in minerals processing, as ferrihydrite has very poor filtration characteristics, and more crystalline phases could be significantly easier to handle. It appears that ZnS has this effect because of its ability to act as a reductant, producing a small amount Fe(II) which in turn favours the formation of goethite. We are continuing to investigate the mechanism of this reaction, and are investigating whether other solid-phase reductants might also be used in this way. PhD student Mitch Loan completed his project on ferrihydrite crystallization control, and took up a post-doctoral position at the University of Limerick in September 2003. During the year, Mitch continued to collaborate with Prof John Cowley at Arizona State University in a detailed study of the iron oxy-hydroxide known as schwertmannite. Nanodiffraction and high resolution TEM experiments have suggested that the structure of schwertmannite may be different from that which has been widely reported in the literature. The effect of molybdate ion on phase transformation of ferrihydrite to hematite has been an important area of research since we discovered that a new iron oxyhydroxide phase can be formed with molybdate incorporated into the structure. The study of this new phase is the subject of an Honours project being undertaken by Dale Carroll. Dale is studying how molybdate influences the phase transformations of ferrihydrite in the presence of other common anions such as sulfate and nitrate.

High magnification SEM image showing the hedgehog-like morphology of schwertmannite.
FUTURE WORK
The study of the new iron oxide phase incorporating molybdate will continue, and we will attempt to prepare analogous compounds using similar anions such as chromate, tungstate and vanadate. We also hope to study the properties of the new material to explore any possible applications. Our recent work on schwertmannite has raised some questions about its structure, and we hope to carry on these studies in order to reach a definitive understanding of the schwertmannite structure, along with the structures of related phases that incorporate inorganic anions.

OUTCOMES
- New insight into the little understood structure of schwertmannite.
- We have shown that ZnS can be used to promote transformation of ferrihydrite to more crystalline phases.
- A new iron oxyhydroxide phase has been discovered. This phase has a structure analogous to β-FeOOH, but with molybdate incorporated into the lattice.
Research Projects

These projects are directed more towards fundamental nanochemistry in areas within and beyond of hydrometallurgy. While some of the research conducted was specifically for industry, other projects were directed towards investigating research areas that can be applied to a variety of disciplines and applications.

Gas Hydrates
The project was commenced in 2001, with an extension commencing 2002, and was completed in 2003. This was a collaborative research project with the Woodside Petroleum Foundation and is Commercial in Confidence.

Causes of Growth Rate Dispersion in Lactose Crystallization during Cheese Production
This project was sponsored by Dairy Australia and commenced in 2000. Research into this area has concentrated on improving the knowledge of factors affecting the growth rate dispersion of lactose crystals, utilising the information gained to improve control of growth rate dispersion. This will lead to improved quality of lactose produced, and potentially increase overall growth rates in industrial lactose crystallisers. The project also aims to make available university personnel experienced in lactose crystallisation and growth rate dispersion, so that these researchers can consult with Australian producers. The project was successfully completed in 2003.

Determination of Crystal Structure of EMD
This project, sponsored by HiTec Energy, was a first for the NRI with all the research being conducted with the use of computational molecular modelling. The initial work in this area has led to the successful application for an Australian Research Council - Linkage grant for an Australian Postgraduate Award (Industry). The initial project commenced in December 2002 and was competed in 2003. The results are Commercial in Confidence at this stage.

The collaboration has continued in the form of the APA(I) funded PhD project, where the electrodeposition of manganese dioxide is being investigated using experimental and theoretical methods. This project is focussing on how the nanoscale processes taking place at the electrode surface impact on the bulk properties and battery performance of the EMD.

Control Strategies for Silica Scale in the Solvent Extraction Process of Copper
This project was commissioned by Western Metals Ltd and went over a period of three months. The project consisted of three parts: A survey of dissolved and particulate silica in plant liquors involving a visit to the processing plant near Mt Isa, characterization of residual solids after leaching and characterization of residual solids in the solvent extraction circuit.
Lactose is produced in large amounts as a by-product of the diary industry and has several industrial applications. Lactose is purified by crystallization as $\alpha$-lactose monohydrate; the extent and speed of crystallization is affected by the experimental conditions and in particular by the presence of $\beta$-lactose. In water, $\alpha$- and $\beta$-lactose are in equilibrium, and $\beta$-lactose is the most abundant isomer. However, the $\alpha$-form is much less soluble. For this reason $\alpha$-lactose is usually precipitated from lactose solutions. The surface structure of different crystal faces and the energetics of $\beta$-lactose incorporation in $\alpha$-lactose monohydrate crystals have been studied to understand the factors that affect the growth of the crystals.

Lactose-water interactions at the crystal surface are expected to play a significant role in determining the surface morphology and energetics as lactose molecules have several hydroxyl groups capable of forming hydrogen-bonding interactions. For this reason, molecular dynamics simulations of the crystal-water interface were undertaken.

The computer simulations indicate that, in water, the first two layers of the (010) crystal surface undergo a large reconstruction (Figure 1). This reconstruction is driven by the tendency of the lactose molecules to expose one of the hydrophilic OH groups to the solvent. Adsorption of $\beta$-lactose on this crystal surface is predicted to be energetically unfavorable. The (0-10) crystal surface is rather hydrophilic and does not reconstruct significantly in water. Adsorption of $\beta$-lactose on this crystal surface is predicted to be energetically favorable; furthermore, the adsorption of even a few molecules of $\beta$-lactose is predicted to prevent the growth on this crystal face. These results provide an explanation for the observation that $\beta$-lactose has only a small effect on the (010) face, while it completely stops crystal growth on the (0-10) face.

Further simulations are in progress to characterize at the atomic level of resolution the structures of the other crystal faces that are observed experimentally and to study the energetics of $\beta$-lactose incorporation.

Figure 1. (010) surface of $\alpha$-lactose monohydrate. The red and blue colours highlight the herringbone reconstruction.
BACKGROUND
In the past two decades there has been an explosion of research into the use of a novel form of carbon, namely fullerenes and carbon nanotubes. The discovery of a third form of carbon, apart from graphite and diamond, by Smalley, Kroto and Curl have generated waves of discoveries as the properties of these nanostructures are being constantly investigated. The discovery of nanotubes of carbon (CNTs) by Ijima in Japan, has generated much interest for their novel properties. The tensile strength of carbon nanotubes has been measured to be stronger than steel of similar dimensions. Carbon nanotubes have been shown to possess superconductivity properties if properly doped with potassium. CNTs can be functionalised and added to an existing AFM to obtain high resolution (atomic and molecular) and surface force maps of special functional groups on surfaces and membranes. Carbon nanotubes have been shown to be a good absorbent for gases like H₂, CH₄, and C₄H₁₀ and may become the backbone of a national Hydrogen economy as the main impediment to establishing the latter has been the storage factor. With some preliminary research showing promise for hydrogen storage in Nanotubes, this area is being researched actively to improve the gas adsorption characteristics of CNTs.

ACTIVITIES
In the past year we have finished the plans for the chemical vapour deposition, (CVD) chamber and have secured some laboratory space to perform experiment on Nanostructures. A small scale CVD system was tested and carbon nanotubes have been successfully made with using ethylene gas with both iron or nickel based catalysts.

There are very exciting prospects for the new technology and it will have impacts in various areas of Science and Industry.

We have been granted seed funding of $15,000 for the manufacture of Nanocarbons and nano-diamonds by Woodside Corporation.

The collaboration with Sir Charles Gairdner Hospital has continued and we have been able to make some well-defined nanoparticles of stibnite. These nanoparticles are generally used to exchange with radioactive Tc to form Tc-99m antimony sulphide in a hot-cell and then they can be used for early diagnosis of lymphodema or melanomas.
In the Nanostructure Research Laboratory we have been successful in synthesising a range of nanoparticles with different types of materials. Metallic and semiconductor particles of nanometre sizes and varying shapes have been made.

**FUTURE WORK**

Based on the initial success of our method of producing carbon nanotubes, the synthesis by CVD will be optimised and the Woodside work is anticipated to yield some interesting results.

On the Nanoparticles synthesis front, optimisation of the technique will be pursued and ways to scale up production will be investigated. Other groups in WA have indicated interest in some of our products and discussions about collaboration are underway.
OBJECTIVES
Our goal has been the development and utilization of powerful computer modelling tools in the simulation of molecular and crystal systems. The techniques that have been implemented are freely available in the software package GDIS, which can be obtained from the web site: http://gdis.sourceforge.org. The main focus for development has been on the computation and visualization of bulk and surface properties of crystalline systems.

ACTIVITIES
Two useful representations of a surface, the molecular and accessible surface, are computable in GDIS. Both of these are defined in terms of a probe of desired radius in contact with the atoms on the surface of the material. Important properties can be encoded into the molecular surface. For example, the closest atom to the surface yields information as to which surface species are in contact with the probe. In addition, colouring the surface according to the perpendicular height (Figure 1a) gives an ideal “AFM” image. Also, mapping the electrostatic potential (Figure 1b) can be a useful aid in predicting the location and binding strengths for adsorption species.

A project examining the structure and defects in electrolytic manganese dioxide (EMD) was undertaken. Visualization of known stacking faults (Figure 2 – a ramsdellite/pyrolucite stacking fault) enabled theoretical models of the defect structure of manganese dioxide to be constructed. This was achieved by comparing the formation energies of the important stacking faults to establish the relative likelihoods of occurrence. Postulated repeat cells, involving specific concentrations of defects, were then constructed and used to compute a corresponding diffraction pattern. These calculated patterns were then compared to experimental patterns.
OUTCOMES AND FUTURE WORK

A paper utilizing GDIS for the visualization of complex organic solids has been published. Two other papers, based on the computation and visualization of surface properties, have also been submitted. It is anticipated that work on the defect structure of manganese dioxide will also be published. Finally, it is also intended to further enhance the surface code visualization by implementing additional property mappings such as curvature and electron density iso-surfaces.
OBJECTIVES

In order to understand chemical and physical processes at the nanoscale it is important to have a clear picture of what is occurring at the atomic level. Our objective is to develop the means by which computer simulation can be applied to problems at this length scale and to utilize these tools to optimise the design nanochemical systems.

ACTIVITIES

The key problem that prevents the use of computational methods for the study of large systems is the rate at which the cost increases as the simulation gets larger. If the number of atoms is $N$, then the demands of a forcefield method increase as $N^2$, while those of more accurate quantum mechanical methods rise as $N^3$. In the last year we have been working on the implementation of techniques that make the expense of both simulation methodologies scale only linearly with the system size, thus making it feasible to study key systems in nanotechnology. Below we highlight two studies that have been performed using some of these developments.

(i) Hydrogen storage in carbon nanotubes

Hydrogen is potentially the most environmentally sustainable fuel of the future since it only yields water on combustion. However, to make this a reality a means of efficiently storing hydrogen in a safe, lightweight form must be found. Our work has been investigating what happens when hydrogen is adsorbed into carbon nanotubes. If nanotubes with a small radius are used then it appears that hydrogen can react with the host material and that this leads to a dramatic change in shape that has important consequences for its ability to store physisorbed hydrogen within the pores.

(ii) Minerals for quantum dots

Recent interest in nanotechnology has led to a quest to understand the properties of particles of dimensions of just a few nanometres, where there may be significant alterations in the electronic behaviour. Because of their semi-conducting properties and tuneable band gaps, the sulphides of lead, cadmium and zinc have attracted particular attention as examples of quantum confinement. We have performed a study of the structure and electronic properties for nanoparticles of the mineral galena (PbS).
A key issue for any nanoparticle is the nature of the morphology. Given that lead sulphide adopts the rock salt structure, we have initially considered particles exhibiting the dominant (001) surface. However, for the larger particles we have also included the (110) surface, as the other particularly stable non-polar surface cleavage plane, in order to consider spherical and ellipsoidal morphologies. Simulations show that even at small particle sizes the cubic morphology is the energetically favoured one. There is also a strong correlation between the particle morphology and the band gap, with the cubic material having the largest value.

If quantum dots are to find technological application it is crucial to find a means of stabilising them to prevent aggregation, while leaving their properties unperturbed. Our results suggest that small PbS particle can be incorporated within zeolitic frameworks to create regular arrays, and that because the key electronic levels of lead sulphide lie within the band gap of SiO₂ the electronic confinement is maintained.

FUTURE WORK

One of the key challenges is to be able to calculate the spectroscopic properties of nanoscale systems for experimental identification and to explore many of their potential applications. Work is underway to explore the use of time-dependent quantum mechanics in order to study excited states of quantum dots and thereby to determine their optical behaviour.

OUTCOMES

- Linear scaling calculations for nanotechnology forcefields implemented
- Thermodynamics of hydrogen chemisorption on (n,n) carbon nanotubes has been predicted
- The variation of stability and band gap with the size and shape of lead sulphide semiconducting nanoparticles has been determined.
OBJECTIVES

Most processes of industrial significance occur at surfaces e.g. precipitation, scale formation, dissolution. In order to simulate these processes successfully, a realistic description of these surfaces and their interactions with solution and foreign molecules and ions is needed. Our objective is to develop the tools and theories to make this possible.

ACTIVITIES

In 2003, great strides to accomplishing the objective have been achieved via the incorporation of surface simulation tools into two of the computer codes devopmed in the NRI: GULP and GDIS. This new functionality has been demonstrated in some of the projects that have been undertaken in the NRI in 2003, listed below:

(i) Simulating calcite surfaces: scale to gallstones

Scaling in industry results when particles grow on, or adhere to, the surfaces of equipment. A very common culprit is calcite. Scale formation causes many problems from equipment failure to loss of product. At the very least, scale formation increases the cost of running and maintaining equipment. Thus, it is clear that controlling or mitigating the formation of scale is an important part of any industrial process.

The human body also suffers from a similar problem, in this case the formation of kidney and gallstones. The primary constituent of the latter is cholesterol monohydrate (~80 wt %); however, significant levels of calcium carbonate (~15 wt %) and calcium phosphate (~ 3 wt %) are also present. The coexistence of these minerals with cholesterol deposits suggests a synergistic influence of one crystalline phase on the other, and may be an important factor in nucleation and growth under physiological conditions.

Our interest in calcite scaling under industrial conditions has led us to undertake a study into the surface structures of calcite. This required the development of a high quality set of interatomic potentials. These potentials were found to predict a surface reconstruction of the basal plane of calcite, unlike the other commonly used potentials in the literature. This reconstruction has been observed to occur experimentally using LEED, and our calculations provide an atom-level picture of the phenomenon.

Armed with these potentials, we have simulated the interactions between cholesterol monohydrate crystals and the calcite basal plane. Both geometric and chemical interactions were found to influence the alignment of ions and molecules at the boundary of these two different crystalline materials. Perhaps not surprisingly, the presence of interfacial water molecules plays a key role in mediating the repulsive interactions associated with bringing ionic and neutral surfaces together. Most significantly, it was found that it is more energetically favourable for cholesterol monohydrate crystals to nucleate on calcite than on cholesterol monohydrate itself. This correlates well with in situ AFM studies, where we have demonstrated experimentally that the basal plane of calcite can serve to catalyze the precipitation of cholesterol monohydrate from bile solutions.
(ii) Solvation and the morphology of crystals

One of the most important properties of a crystal in an industrial context is the morphology i.e. its size and shape. It is well known that the solvent plays an important role in this process but to date there is no simple way to incorporate this into molecular modelling calculations. We are developing an algorithm called COSMIC to allow this. Although the algorithm is not yet fully complete, we have used an interim version to calculate the surface energies of the faces of sphalerite in the presence of water. All surface energies decrease upon solvation, which is expected as the surface regains some of the energy it lost on cleavage in a vacuum by interacting with the solvent. The key finding is that the amount the surface energy reduces on solvation is dependent on the face e.g. the (110) face has its surface energy reduced by just 0.06 Jm$^{-2}$, whereas the S terminated (111) face is reduced by 0.51 Jm$^{-2}$. Thus in the “wet” morphology, the (100) and (111) forms are also expressed, giving a description of sphalerite morphology that is much closer to that observed experimentally.

Morphology of sphalerite (a) in the absence and (b) in the presence of water.

FUTURE WORK

The COSMIC algorithm will be fully implemented and tested on systems of pharmaceutical interest. Surface simulations employing the GDIS and GULP codes will now focus on calcite in the presence of calixarenes to give an atomic level description of the results of the atomic force microscopy experiments undertaken at the NRI.

OUTCOMES

- The surface reconstruction of the basal plane of calcite has been successfully modelled for the first time
- An atomic level description of the role of calcite in promoting the nucleation of cholesterol has been obtained
- Surface solvation can now be accounted for using the COSMIC algorithm.
The students within the NRI are as important to the Institute as its research staff. They bring to the Institute a willingness to learn, expand and share knowledge. It is through interactions between all members of the Institute that new ideas and innovation are generated.

The following students completed their Masters during 2003

<table>
<thead>
<tr>
<th>Name</th>
<th>Project Title</th>
<th>Supervisors</th>
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<tbody>
<tr>
<td>Ayon Guha</td>
<td>Influence of amino acids on the crystallographic character of calcium carbonate</td>
<td>Assoc Prof A van Riessen Assoc Prof MI Ogden</td>
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<tr>
<td>Davlin M D Chokazinga</td>
<td>Coordination Studies of Inositols with Aluminium and Related Cations</td>
<td>Dr M Mocerino Assoc Prof B van Bronswijk</td>
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The following students completed their Honours thesis during 2003

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<tr>
<th>Name</th>
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<tr>
<td>Jade Pettersen</td>
<td>An approach towards calixarene nanotubes</td>
<td>Assoc Prof MI Ogden Dr M Mocerino</td>
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<tr>
<td>Joanne Crocker</td>
<td>Synthesis and application of 1,3-alternate calix[4]arenes in the extraction of heavy metals</td>
<td>Assoc Prof MI Ogden Dr M Mocerino</td>
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</table>

The following students commenced their Honours thesis during Semester 2, 2003

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<tr>
<th>Name</th>
<th>Project Title</th>
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<tbody>
<tr>
<td>Dale Carroll</td>
<td>Incorporation of Molybdate anion into Iron-Oxyhydroxide Structures</td>
<td>Dr Bill Richmond Prof Gordon Parkinson</td>
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PhD Students

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<tr>
<th>Name</th>
<th>Project Title</th>
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<tr>
<td>Kristy Blyth</td>
<td>Causes of growth rate inhibition in lactose</td>
<td>Prof GM Parkinson Assoc Prof MI Ogden</td>
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<tr>
<td>*Wannapa Boonwanich</td>
<td>Inhibition of crystal growth of sparingly soluble salts (written up)</td>
<td>Prof GM Parkinson Assoc Prof MI Ogden</td>
</tr>
<tr>
<td>Damien Carter</td>
<td>Mechanisms of dye incorporation into potassium sulphate</td>
<td>Assoc Prof AL Rohl Assoc Prof MI Ogden</td>
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<tr>
<td>Ryan Chester</td>
<td>Calixarenes as Potential Ionophores for Ion-Selective Electrodes</td>
<td>Dr Mauro Mocerino Assoc Prof MI Ogden Assoc Prof R De Marco Prof GM Parkinson Assoc Prof MI Ogden</td>
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<tr>
<td>Amal Freij</td>
<td>Crystallization of Lactose from Whey and Permeate</td>
<td>Assoc Prof MI Ogden</td>
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<tr>
<td>Djwantoro Hardjito</td>
<td>Physical Properties of Geopolymer Concrete</td>
<td>Prof B V Rangan, Prof GM Parkinson, Dr P Kong</td>
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<tr>
<td>Robert Herman</td>
<td>The Synthesis And Bioactivity Of Some Novel Biphenyl Xanthone Derivatives With Antidiabetic Activity</td>
<td>Dr Mauro Mocerino, Assoc Prof E Helmerhorst</td>
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<tr>
<td>Tung Hoang</td>
<td>Effect of Substrates on Scale Formation</td>
<td>Assoc Prof Andrew Rohl, Dr M Ang</td>
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<tr>
<td>Michael Kiriazis</td>
<td>Gibbsite-oxalate interactions in the Bayer refinery scale growth</td>
<td>Prof GM Parkinson, Dr Tony Leong (QAL)</td>
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<tr>
<td>Felicia Lee</td>
<td>Interfacial chemistry of the Bayer process</td>
<td>Prof GM Parkinson, Assoc Prof B van Bronswijk, Dr MM Reyhani, Dr C Vernon (CSIRO)</td>
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<tr>
<td>Mitch Loan</td>
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<td>Prof GM Parkinson, Dr OMG Newman (Pasminco), Dr JB Farrow (CSIRO)</td>
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<tr>
<td>Jennifer Lowe</td>
<td>Fundamentals of scale formation</td>
<td>Prof GM Parkinson, Assoc Prof AL Rohl, Dr P Smith (CSIRO)</td>
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<td>Matthew McIlldowie</td>
<td>Chiral Calixarenes</td>
<td>Dr Mauro Mocerino, Assoc Prof MI Ogden</td>
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<tr>
<td>Jonathon Morton</td>
<td>Better Batteries via Controlling the Properties of Electrolytic Manganese Dioxide</td>
<td>Assoc Prof MI Ogden, Assoc Prof AL Rohl, Prof M Nicol (Murdoch), Dr Chris Ward (HiTec Energy)</td>
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<tr>
<td><strong>Stefanus Muryanto</strong></td>
<td>The role of impurities and additives in the crystallization of gypsum</td>
<td>Prof GM Parkinson, Dr M Ang</td>
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<td>Gianluca Paglia</td>
<td>Determination of the structure of gamma alumina using empirical and first principles calculations with supporting experiments</td>
<td>Assoc Prof AL Rohl, Assoc Prof C Buckley, Assoc Prof A van Riessen</td>
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<tr>
<td>Matthew Rowles</td>
<td>Interfacial bonding in alkali-activated aluminosilicate polymers</td>
<td>Prof GM Parkinson, Prof B O’Connor, Prof P McCormick, Prof V Rangan</td>
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<tr>
<td>Mike Shaw</td>
<td>The adsorption of oxalate seed poisons onto sodium oxalate</td>
<td>Prof GM Parkinson, Dr R Cornell (Alcoa)</td>
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<tr>
<td>Howard Smith</td>
<td>Removal of trace metals from Bayer process wastewater</td>
<td>Prof GM Parkinson, Dr G Sipos (Alcan Gove Pty Ltd), Mr S Healy (Alcan Gove Pty Ltd)</td>
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<tr>
<td>Name</td>
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<tr>
<td>*Suharso</td>
<td>Investigation of the crystallization of sodium borate</td>
<td>Prof GM Parkinson</td>
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<td>Assoc Prof MI Ogden</td>
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<td>Marthin Dody Josias</td>
<td>Behaviour and Strength of Geopolymer Concrete Members</td>
<td>Prof B V Rangan</td>
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<td>Sumajouw</td>
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<td>Prof GM Parkinson</td>
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<td>Steenie Wallah</td>
<td>Long-Term Properties and Durability of Geopolymer Concrete</td>
<td>Prof B V Rangan</td>
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<td>Karsten Winter</td>
<td>Experimental Approaches to Biomineralization</td>
<td>Assoc Prof A Rohl</td>
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<td>Yennhi Vo</td>
<td>The effects of additives on crystal growth rates and morphology of gibbsite</td>
<td>Prof GM Parkinson</td>
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<td>Dr M Mocerino</td>
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Attendees at the 8th Annual Nanochemistry Research Institute and Parker Centre Student Seminar Day
PhD Project: Calixarenes as potential ionophores for Ion-selective Electrodes

OBJECTIVES
Ion-selective electrodes (ISE) are electrochemical sensors that enable the monitoring of a primary ion in the presence of various interfering ions. The primary focus of this project is to incorporate calixarenes into plasticised poly-vinyl chloride (PVC) membranes for the detection of heavy metals such as thallium and mercury. The calixarene acts as the ion-sensing medium in the membrane through the process of ion/ligand complexation. The calixarene’s structure/functionality influences the ion binding properties, which in turn affects both sensitivity and selectivity in ISEs. Commercially available ISEs often provide a cheaper and quicker analysis over the more conventional methods such as ICP and AAS.

ACTIVITIES
Traditionally the majority of plasticised PVC ISEs use the internal filling solution (IFS) method as the preferred technique. Mixed results were obtained using this method in initial trials. Recently a new approach involving “coated wire” type electrodes has been pursued. The new method is currently being extensively tested. The technique incorporates many parameters, which need to be optimised to gain a steady electrode response. In addition to the electrode studies, synthesis and characterisation of previously studied and new calixarenes is continuously undertaken.

OUTCOMES
The vigorous testing of the different electrode parameters has finally yielded an electrode with a steady response of 59.7 mV decade\(^{-1}\), which is only 0.5 mV off ideal. The same calixarene used in the IFS method gave a response of 56.9 mV decade\(^{-1}\). The new electrode also reaches a steady response after only a few seconds compared to a few minutes for the IFS method. The new technique looks to be a superior method for electrode preparation. Some interesting properties of the tetra-isopropylcalix[4]arene have also risen from its characterisation. The compound crystallises with two different types of crystal packing, depending on the incorporation of a solvent molecule. The incorporation of chloroform into the crystal (see Figure) is interesting in that it holds the chloroform solvent up to temperatures of 150 °C, well above its boiling point of 61 °C. Other chloroform solvates with calixarenes have been discovered, but none have been reported where the molecule resides outside the calixarene cavity. Some of these results are to be presented at the 29th International Symposium on Macroyclic Chemistry (July 2004). A tetraisopropyl substituted p-tert-butylcalix[6]arene has also been synthesised and partly characterised.

FUTURE WORK
Future work will be conducted duplicating the current coated wire electrode response and also characterising it further. Characterisation of the electrode will consist of selectivity, pH, and lifetime tests. Other plasticisers may also be incorporated into the membranes to see the effect each has on the response. The membrane will also be characterised further using EIS, AFM, SANS and possibly SIMS. An AINSE grant has been awarded (commencing 2004) to allow analysis time at ANSTO’s facilities to access the SANS instrument. Future work will also be carried out on the current range of calixarenes to determine their metal binding properties.
The aim of this project is to use macrocyclic systems as scaffolds to arrange crystal growth modifying moieties such that selective interaction with crystal faces is achieved. The macrocycles selected are polyphenols named calixarenes. The synthetic chemistry of these compounds is well established and versatile, enabling us to produce a wide range of potential crystal growth modifiers. The crystal systems under investigation include gibbsite and calcite. Over the past 12 months, the project has focussed on the solution phase properties of the macrocyclic additives.

Solution phase interactions of tetra-proline calixarene (1) with a series of small neutral water soluble alcohols were thoroughly investigated by nuclear magnetic resonance spectroscopy (NMR). Previously, the inclusion of \( t \)-butanol by \(^{13}\)C NMR was extensively investigated. It was found that the calixarene proline derivative complexed with \( t \)-butanol in water producing splitting of peaks in carbon NMR spectra. The intensity of the split peaks relates to the amount of \( t \)-butanol in solution. Such well defined binding of an alcohol in an aqueous solution is a significant discovery. The study was extended to a wider range of small, water soluble, neutral alcohols. The different guests include methanol, ethanol, propanol, isopropanol and 2-butanol, with the proline calixarene acting as the host. Results from the upfield shifts in \(^1\)H NMR suggest that the aliphatic moiety of the guests is selectively included into the hydrophobic cavity of the calixarene, while the more hydrophilic OH group interacts with the proline groups.

The potential phase transfer or other chiral recognition applications of proline calixarene were further investigated. NMR was used to gauge proline calixarene’s potential for selectively binding different enantiomers. Not only a shift in \(^1\)H NMR was observed, but splitting also occurred due to the formation of two diastereomeric complexes with the proline calixarene.

Thesis preparation is now underway, along with final work on the crystal growth aspects of the project.

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\begin{align*}
\text{HO} & \quad \text{N} \\
\text{CHO} & \quad \text{O} \\
\text{N} & \quad \text{CO} \\
\text{OH} & \quad \text{OH} \\
\end{align*}
\]

(1)
PhD Project: Mechanisms of Dye Incorporation into Potassium Sulphate

OBJECTIVES
A dual approach, combining experimental and molecular modeling studies, is being employed to work systematically towards a deeper understanding of the mechanism of dye incorporation.

ACTIVITIES

Experimental studies
Experimental studies have focused on using in situ optical microscopy to monitor crystal growth.

Molecular Modelling Studies
The interactions of ortho-sulfonated aniline (OSA) and benzene-sulfonate (BS) with various potassium sulfate surfaces has been examined using molecular mechanics and density functional techniques.

OUTCOMES

Experimental studies
Experiments were conducted to measure the growth rates of potassium sulfate faces in pure solutions, and in the presence of dyes. A number of different conditions have been examined. Results to date suggest, for the conditions examined, there is not a distinct change in growth rate after the addition of acid fuchsin.

Molecular Modelling Studies
Molecular mechanical docking calculations were completed using OSA and BS docked on potassium sulfate. Whilst results were in broad agreement with experiments, a few inconsistencies remain. Density functional calculations were employed to determine whether the differences are due to inaccuracies in calculating surface-dye interactions. Results are currently being processed, but suggest the model of incorporation may be too simple.

FUTURE WORK
All results from molecular modelling calculations and experimental studies have to be analysed and finalised. These results will then be reported in thesis form.

OTHER
During the year, talks were presented at the NRI annual student seminar day and for the Department of Applied Chemistry at Curtin University.

One of the stable docked configurations of BS in potassium sulfate calculated using quantum mechanics (left) and interatomic potentials (right)
Desilication product (DSP) is paradoxically both useful and also a problem in the Bayer process, which is used to produce alumina. DSP is an aluminosilicate compound, comprised of two main phases, sodalite and cancrinite. Most DSP is precipitated prior to the digestion phase, and has an important role in removal of impurity anions from the closed process circuit. Silica not precipitated as DSP in this initial stage remains in the process circuit, and can precipitate as scale in heat exchangers and on pipes, representing a significant cost to industry.

The objectives of this research program include a fundamental investigation of formation of DSP under Bayer conditions. This encompasses kinetic studies and characterisation of compounds formed in the presence of common process anions, as well as identification of conditions or inhibitor compounds able to reduce the kinetics of formation. A combined modelling and experimental approach has been taken in order to achieve these aims.

Modelling of incorporation of impurity anions into DSP has continued during this year, with extension of the already completed molecular mechanics calculations examining binding energies. This further research has included molecular dynamics calculations allowing study of the interactions between the impurity anions and DSP over time, and also quantum mechanical calculations. Additional structural determination experiments utilising the high resolution powder diffractometer at the ANSTO Lucas Heights facility were undertaken, with an improvement in the data collected from previous experiments. Study of anion-containing DSP samples by solid state NMR was also conducted at the ANSTO Lucas Heights facility, following on from early samples analysed at the University of Western Australia. The mechanistic pathway of DSP formation has been studied during this year by TEM and XRD analysis. DSP samples prepared in the presence of different anions, and using different clay precursors, have been examined.

Further NMR experiments at the ANSTO Lucas Heights facility will be undertaken this year. Molecular dynamics calculations of anion-DSP compounds will also continue. Further work on the mechanism of formation of DSP, using both TEM and isotopic aluminium studies combined with accelerator mass spectrometry, will be conducted.
PhD Project: Effect of Substrates on Scale Formation

OBJECTIVES

The overall aim of this research is to develop a method for studying scale formation and to determine the relationship between scale growth and the presence of impurities or additives as well as typical process parameters in order to understand the scaling mechanism and propose optimized conditions for industrial processes to control scale formation.

The approach of the research is as follows:

- Derive some correlations between the rate of scale growth and the process parameters such as temperature, flowrate, pipe diameter, using a pipe flow system.
- Investigate the effects of some impurities and organic substrates on scale formation.
- Construct a quartz crystal microbalance to conduct an *in situ* study of the scale formation in pipes.
- From the results, give some recommendations for scale control in industrial processes.

ACTIVITIES

Experiments on scaling in pipes have been undertaken using a previously constructed flow system. The results have been analysed and some conclusions have been drawn.

A multiple-flow system that permits continuous study of scale formation is being developed.

A quartz crystal microbalance system used for investigating calcium sulphate scaling is being constructed and tested.

OUTCOMES

A paper on my research has been published in the Proceedings of the 31st Annual Australasian Chemical Engineering Conference (Adelaide).

A poster revealing my experiment results was presented at Chemeca2003 (Adelaide) and at the Exhibition for the 21st Anniversary of Chemical Engineering Department at Curtin University (Perth).

Two papers have been submitted to the 10th Asian Pacific Confederation of Chemical Engineering Congress (Japan) and the 32nd Annual Australasian Chemical Engineering Conference (Sydney).

FUTURE WORK

A seminar and a poster are to be presented at the Rottnest Symposium in June 2004.

OBJECTIVES
The preparation of a variety of C4 symmetric calix[4]resorcinarenes by the acid catalysed (boron trifluoride) condensation of asymmetric resorcinol units and aldehydes has been thoroughly investigated. However, the reaction produces a racemate that must be resolved before the enantiomers can be applied as chiral ligands for catalysis and phase transfer separations. The objective of the current research program is to resolve the racemic mixtures using a variety of methods. The absolute stereochemistry of the resorcinarenes can then be determined. The investigation and application of these chiral resorcinarenes has led to collaboration with Professor Harry Heaney of Loughborough University in the UK.

ACTIVITIES AND OUTCOMES
The resorcinarenes were resolved via the preparation of the diastereomeric amide derivatives of the type (1). The single crystal x-ray structure of the C-propyl resorcinarene amide derivative has been obtained. The suite of amide derivatives has been thoroughly characterised. The tetra-camphorsulphonyl (2) derivatives have also been prepared to determine the absolute stereochemistry of the resorcinarene structures. A single crystal suitable for x-ray analysis has been grown and is currently being investigated.

FUTURE WORK
The characterisation and application of the resolved diastereomeric derivatives and their parent compounds is well underway. Their enantio-discrimination with respect to small chiral guest molecules is to be investigated by nuclear magnetic resonance. The preparation of metal complexes of the chiral ligands is also to be investigated with an aim to using them as chiral catalysts.
Western Australian Nanochemistry Research Institute
By far the biggest activity within the NRI during 2003 was the preparation and submission of the application for Western Australian Nanochemistry Research Institute (WANRI) under the State’s Centre of Excellence program to the Office of Science and Innovation. The business plan and application for this proposal were developed to formalise and focus the nanochemistry research activities within Western Australia, and to enhance the reputation of the State as a national and world leader in the niche area of nanochemistry. WANRI will bring together the researchers from the NRI, Curtin University; School of Biomedical and Chemical Sciences, UWA; Department of Physics, UWA; and the Murdoch University Surface Analysis Laboratory (MUSAL).

Premier’s Science Award
Congratulation to Dr Mauro Mocerino who received the Premier’s Prize for Excellence in Science Teaching in 2003. This award recognises the special skills and expertise of teachers in the delivery of science education across the University and TAFE sectors.

Recruitment
The recruitment of internationally recognised researchers has proven to be extremely successful in 2003. The NRI was fortunate enough to be able to recruit Professor Julian Gale, previously a Reader in Theoretical and Computational Chemistry at Imperial College London. Professor Gale was awarded the inaugural Premier’s Research Fellowship worth $1 million over four years. This has greatly enhanced the Computational Molecular Modelling Facility, which is sure to further enhance the capabilities and reputation of the NRI and Curtin. Other recruitments made during 2003 will further strengthen the research capabilities of the NRI. Dr Alistair Fletcher was seconded from CSIRO and Professor Kate Wright from University College London joined the NRI as an Adjunct Professor.

Collaboration
Collaborations with national and international partners is a core component to the success of the NRI. In 2003, collaboration between A/Prof Andrew Rohl and Bart Kahr, University of Washington, Seattle, has continued on probing the interactions that lead to dye inclusion crystals. A/Prof Rohl has also been collaborating with Jennifer Swift, Georgetown University, Washington DC, on Modelling the Crystal Growth of Cholesterol on Calcite. A/Prof Mark Ogden and Dr Mauro Mocerino have been collaborating with Allan White and Brian Skelton from the University of Western Australia on the Structural Chemistry of Calixarene Supramolecular Assemblies. Prof Julian Gale has continued strong collaboration with international researchers such as German Sastre, Istituto de Tecnologia Quimica, Valencia; Andrew Walker, Ben Slater and Kate Wright, Royal Institution of Great Britain; and Alexander Shluger, University College London, to mention a few.

Grant Successes
During 2003, several grants and industry contracts were awarded to the researchers within the NRI. Congratulations to Prof Gordon Parkinson and Prof Kate Wright, who in conjunction with A/Prof Craig Buckley, Department of Applied Physics, and A/Prof Tim St Pierre, University of Western Australia, were awarded an Australian Research Council - Discovery Project grant for the project entitled “Ferrihydrite: Fundamentals of a Natural Nanomaterial”. Congratulations to A/Prof Mark Ogden, who in conjunction with Dr Heather Benson and Dr Yan Chen, Department of Pharmacy, Dr Neil Rothnie, Monash University, Dr Peter Taylor and Dr Steve Wilkinson, Chemistry Centre, were awarded an
Australian Research Council - Linkage Project grant for the project entitled “Micro- and nano-particulate delivery systems for chemical and biological weapons: physical characterisation and risk assessment”. Congratulations also to A/Prof Andrew Roh, A/Prof Roland De Marco and A/Prof Craig Buckley, Department of Applied Physics, who were awarded an Australian Research Council - Discovery Project grant for the project titled “Probing the interfaces of electrochemical sensors”.

The NRI also became part of two more CRCs in 2003; the Australian Biosecurity Cooperative Research Centre (AB-CRC) and the Centre for Sustainable Resource Processing (CSRP). The AB-CRC includes organisations such as CSIRO Livestock Industries, Australian Animal Health Laboratory, other universities, and various Commonwealth and State Government agencies. This venture provides a critical mass of multidisciplinary expertise to help protect Australia from emerging infectious diseases. The CSRP aims to create new methods to produce minerals and metals in ways that benefit the community, the environment and industry. This will be achieved by finding technical solutions for progressively eliminating waste and emissions in the materials cycle, while enhancing business performance and meeting community expectations. Research partners include Curtin University, CSIRO Minerals, ANSTO, Central TAFE (WA), other Australian universities, and various Commonwealth and State Government agencies.

Bid for Parker III
In 2003 Round 9 CRC Program guidelines were released and NRI participated in the preparation of the bid for Parker CRC for Integrated Hydrometallurgy Solutions. This Centre will be based on the strong foundation established in the existing A J Parker CRC for Hydrometallurgy, in which NRI is a core partner. The bid will be finalised and submitted in June 2004.

Electron Science Valley
During 2003, the NRI has been engaged as one of the core partners in the proposal under the State scheme for a Western Australian Major Research Facility to become Western Australia’s Electron Science Valley (ESV). Electron Science Valley is the revolutionary integration of microelectronics, nanochemistry, photon and bio based sciences, and nanotechnology to enable novel materials with extraordinary new properties that will underpin the realisation of new components and systems as part of a growth strategy for an emerging economy based on an entirely new frontier of information and communications technologies – newICT. Electron Science Valley is based on an existing $85 million platform created by the innovation of research leaders from Western Australia’s four Universities. An impressive partnership between over 30 national and international universities, institutes and companies brings the necessary skills and infrastructure to support Western Australia’s strengths.

Student Seminar Day
The 8th Annual Nanochemistry and Parker Centre Student Seminar Day was held again this year and with Worsley Alumina and the Parker Centre generously sponsoring the event. There were representatives from a diverse range of companies, including BHP Billiton, Worsley Alumina, Alcan Australia, Nalco Chemicals, CSIRO and MERIWA. The presentations were again of the highest quality and the students did an excellent job of demonstrating the level of commitment they have to their studies and the high quality achievements they have attained through their studies within the NRI.

Mitsubishi Visit
In February 2003, three executives from Mitsubishi visited Curtin to present the company’s recent work in the development and production of fullerenes - intricate nanocarbon molecules that have an array of industrial applications - and to discuss the possibility of a research partnership with the Institute and the University. Frontier Carbon Corporation (FCC) - an arm of the Mitsubishi Corporation - plans to be a world leader in nanocarbon products and materials within the next few years. The NRI is currently engaged in discussions with Mitsubishi about research collaboration and we look forward to work with them in this exciting area of nanotechnology and building of a formal partnership.
The NRI has two state-of-the-art facilities, as well as an extensive range of equipment for the wet chemistry laboratories. The Scanning Probe Microscopy Facility and the Computational Molecular Modelling Facility have been built up through grants and industry funding, and are constantly updated and modified to suit the changing needs of the NRI.

**Scanning Probe Microscopy Facility**  
Manager: Dr Manijeh Reyhani

The Scanning Probe Microscopy Facility consists of instruments that provide very high resolution, three dimensional surface topography on an increasing variety of samples and are powerful tools for surface examination. The instrumentation has been built up over the life of the NRI and is now considered to be a world-class facility for research and development. The uniqueness of the Atomic Force Microscopes (AFM) within the Facility stems from their ability to operate under liquids, including the high temperature (up to \(ca\) 100°C) corrosive solutions frequently encountered in industry. The Facility currently has:

- Digital Instruments NanoScope E - contact mode operation in air, simultaneous sample viewing with optical microscope, and with atomic resolution capability.
- Digital Instruments Dimension 3000 – “contact mode” and “tapping mode TM” operation (for viewing soft samples and weakly adsorbed species), simultaneous sample viewing with optical microscope, in situ liquid cell under ambient conditions, phase imaging, for the study of composite materials, magnetic alloys, etc., interparticle force measurement, large sample imaging capability.
- Molecular Imaging PicoAFM - atomic force microscope - sample imaging in controlled gaseous environment (for air sensitive samples, etc.), in situ imaging of samples in corrosive fluids (high and low pH) and at high temperature (up to around 100°C), operation in contact and intermittent contact modes, atomic resolution capability, “Mac Mode TM” operation for controlled measurement of interparticle forces.
- Molecular Imaging PicoSTM - scanning tunnelling microscope - sample imaging in controlled gaseous environment (for air sensitive samples, etc.) with glove box for sample transfer, in situ imaging of samples in corrosive fluids.
- Nikon Optiphot2 optical microscope - double beam interferometry with Mirau objectives, polarising and tilting stages, in situ flowing liquid cells.
Computational Molecular Modelling Facility
Manager: A/ Prof Andrew Rohl

The Molecular Modelling facilities in the NRI provide a cutting edge capability for simulations of solution, bulk and surface process using both quantum mechanical and force-field techniques. It is well equipped for large-scale computations and for visualisation of these results. The facilities include:

- For visualisation, 4x Silicon Graphics workstations and 3x Dell workstations.
- 12 node Beowulf cluster consisting of 600 MHz Dec Alpha processors, plus 2x dual processor 2.4 GHz Xeon machines connected via gigabit Ethernet for running more memory and bandwidth intensive calculations.
- 160 GB file server and secure firewall/mail/web server

The primary tool used to visualise computational results is the software called GDIS, developed in-house by Dr Sean Fleming. We also use commercial software such as InsightII, Cerius² and Materials Studio. The simulation codes we utilise are primarily the GULP, MARVIN and SIESTA academic codes, all of which are developed by researchers within the NRI.

The Molecular Modelling Facility is also a major user of the APAC AlphaServer SC supercomputer facility in Canberra and IVEC facilities in ARRC, Technology Park.
### Name

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<thead>
<tr>
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<td>Ron Swindells, Don Nicklin, Mark Hochen, Alan Johnstone, John Prott, Graeme Bullock and John Prescott</td>
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<td>Peter Holden</td>
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### Dr Robin Batterham

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<td>Laurence Meagher</td>
<td>The University of Melbourne, Victoria, Australia</td>
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| Ray Dagastine | }
The NRI is a core participant in the AJ Parker CRC for Hydrometallurgy, contributes to the Australian Biosecurity CRC, the Sustainable Resource Processing CRC and the WA Energy Research Alliance.

Research linkages and collaborations include the following institutions:

- CSIRO
- University of Queensland
- Imperial College, London
- University College, London
- Royal Institution, London
- University of Oxford, England
- University of Cambridge, England
- Technical University of Delft, the Netherlands
- University of Nijmegen, the Netherlands
- University of York, England
- University of Southampton, England
- Himeji Institute of Technology, Japan
- Washington State University, USA
- Arizona State University, USA
- University of Nebraska in Lincoln, USA

Alliances and collaboration with industry include:

- Alcoa World Alumina
- Mitsubishi Corporation
- Pasminco Pty Ltd
- Worsley Alumina
- Nabalco
- Queensland Alumina
- Alcan
- Western Mining Corporation
- Woodside
- BHP Billiton
- Queensland Nickel
- Anglogold
- Dairy Australia (formerly Dairy Research and Development Corporation)
- Advanced Particle Technology
- McCusker’s Alzheimers Research Foundation
- Sir Charles Gairdner Hospital
- Royal Perth Hospital
- Mitsubishi Chemicals
- GSK
- Pharmacia
- New Millenium Resources
- Pechiney
Publications

Journal Publications

AL Rohl, K Wright, JD Gale (2003) “Evidence from surface phonons for the (2x1) reconstruction of the (1014) surface of calcite from computer simulation”, *American Mineralogist* 88, pp 921 - 925


Conference Presentations


JD Gale “The SIESTA Method and it’s Application to Nanostructures” 5th Canadian Computational Chemistry Conference, Toronto, Canada, July 2003.


JD Gale “Application of SIESTA method to nanoparticles and defects in materials” First Kyoto Workshop on Computational Materials Science, Kyoto, Japan, March 2003.


F Lee, W van Bronswijk, C Vernon, GM Parkinson and M Reyhani “Nanoscale force measurements on synthetic and industrial gibbsite at low and high pH” International Frontiers of Science: Sir Mark Oliphant Conferences; Scaling Down to a Nano-Materials World, Melbourne, Australia, December 2003.

MI Ogden, GM Parkinson, M Singh, C Buckley and J Connolly “Nanoparticles via Delamination of Li/Al Layered Double Hydroxides” Oz Nano 03, Cairns, Australia, November 2003.


GM Parkinson “Crystallization as a Model for Controlling Self-Assembly and Structural Ordering at the Nanoscale” Oz Nano 03, Cairns, Australia, November 2003.


MI Ogden “Nanotechnology Education at Curtin University of Technology” Oz Nano 03, Cairns, Australia, November 2003.


M Mocerino “Getting the most out of Science Labs” 12th Annual Teaching and Learning Forum, Joondalup, Western Australia, February 2003.


**Technical Reports**

GM Parkinson, TD Dincer and MI Ogden “Causes of Growth Rate Dispersion in Lactose Crystallization during cheese production” October 2003 (Confidential)

F Jones, AL Rohl, WR Richmond and T Upson “Dissolved and Particulate silica in the leaching and extraction of copper at Mt Gordon” November 2003 (Confidential)

SD Fleming and AL Rohl “Investigation into the crystal structure of EMD” September 2003 (Confidential)

GM Parkinson, MI Ogden and AJ Freij “Optimisation of the Causticisation of Bayer Liquors Through Crystallization Chemistry – 12 Month Extension AWA 11-1- Final Report” June 2003 (Confidential)

SD Fleming, GM Parkinson, AL Rohl and AP Stanley “Incorporation of Impurities in Gibbsite during the Bayer Process – P625” August 2003 (Confidential)

F Jones “Analysis of Three Gypsum Scale Samples” January 2003 (Confidential)

F Jones “The role of organics on the precipitation of calcium carbonate” September 2003 (Confidential)

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