April 2011

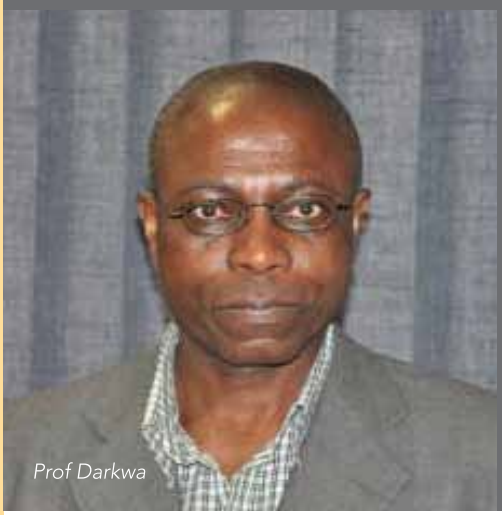
UNIVERSITY OF JOHANNESBURG

# Faculty of Science NEWSLETTER

**2011** - The International Year of **Chemistry is celebrated at UJ**

## UJ co-hosts international conference

One of the first events planned by IUPAC and UNESCO for the International Year of Chemistry was the 40th South African Chemical Institute (SACI) Convention with the theme: Chemistry- The key to Africa's future. The event was held from 16 – 21 January 2011 and was co-hosted by UJ and Wits, although most of the activities took place on the Wits campus. *Prof James Darkwa* from the Chemistry Department was the Chairperson of the Conference Organising Committee for this event, which was a prelude to the official ceremony opening of the International Year of Chemistry and brought chemists from the continent of Africa and the world together to celebrate chemistry. As such the conference was attended by the President of the International Union of Pure and Applied Chemistry, The American Chemical Society President, the President of the Royal Society of Chemistry and the President of the Federation of African Societies of Chemistry. This is a first for any chemistry conference held in South Africa and indeed the whole continent. The scientific programme showcased research activities in all traditional branches of chemistry (Organic, Inorganic, Physical and Analytical) as well as interdisciplinary areas (such as Materials, Nano-science, Bio-inorganic, Green chemistry, Environmental chemistry etc.). It provided a platform for presenting current research work going on in the African continent as well as in the rest of the world. It was an opportunity for chemists on the continent to build links to strengthen the Pan African Chemistry Network (PACN) recently launched in Kenya. The conference was very successful, not only because of the excellent scientific content, but also due to a very good social programme that contributed to the cementing of current and future research collaboration.



*Prof Darkwa*

THIS ISSUE **FOCUSES ON THE DEPARTMENT OF CHEMISTRY.** THE NEXT ISSUE WILL FOCUS ON THE DEPARTMENT OF CHEMICAL TECHNOLOGY

# Research

## In the Department of Chemistry

The main research thrust in the Department of Chemistry at the University of Johannesburg is in the area of catalysis. All the research staff, with the exception of the Analytical Chemistry group, are involved in research into various aspects of this study field. In addition to this focus area all researchers also have other areas of expertise which they are actively building, ensuring a vibrant and dynamic environment in the Department. The industrial focus of various projects has ensured excellent cooperation with industrial partners as well as the creation of a Centre of Excellence in Catalysis by the University Research Committee, which is funded by the University.

The research group of **Prof Bradley Williams** has two main fields of interest. The first deals with physiologically active medicinal compounds, mainly potentially anti-cancer and anti-viral materials. The anti-cancer compounds are porphyrin derivatives, which are more water-soluble than their non-functionalised counterparts, allowing solubility tuning and the possibility of attaching carbohydrate residues to porphyrazines that will enhance their selective uptake by energy-hungry tumour tissues. The anti-viral products are carbohydrate-derived small carbocyclic rings that retain the chirality and much of the functionality of the parent carbohydrate. This allows manipulation of the ring to render it amenable to use as an anti-viral agent. This work relies on a SmI2-mediated radical cyclisation as a key step in the synthetic protocol. The second field of interest is industrially relevant chemistry. This project is funded by industry and government partners, and focuses on industrially relevant, economically important processes. The approach is to investigate the use of polar ligands for use in homogeneous transition metal-promoted reactions. Ligands play a crucial role in the successful outcome of these reactions (e.g. hydroformylation), and the work has neatly demonstrated that polar ligands suitable for use in biphasic media can be used in such reactions. This enables a rapid recycle of the ligand/catalyst system by simple phase separation. Another aspect to this research revolves around metal triflate Lewis acid catalysis, in which metal triflates are used as highly active recyclable entities. This work investigates reactions and products of interest to the commodities chemistry and fine chemistry sectors. Funding for this project is obtained from Sasol, Mintek, THRIP and the NRF.

**The Carbohydrate and Medicinal Chemistry research group** of **Dr Henok Kinfe** focuses on the discovery and development of new compounds which can be used as anti-infective agents of the neglected diseases (TB, Malaria and HIV/AIDS). The research program is divided into three broad areas:

1. Reaction methodology development towards the synthesis of biologically active compounds
2. Synthesis of medicinally important carbohydrate based compounds
3. Synthesis and characterization of metal complexes and nanoparticles as anti-infective agents

Carbohydrates are the most prominently exposed class of molecules that decorate the surfaces of all living cells. These carbohydrates having flexible chains and many potential binding sites are involved in intercellular communications of biological systems such as cell-cell recognition. Such interactions play important roles in

Prof Wiiliams and group

*Dr Kinfe and group*

biological processes such as fertilization, embryogenesis, immune responses, nervous system development, hormone activities, maintenance and pathogenesis of tissues, viral and bacterial infections and cancer metastasis. If success in the utilization of the potential of carbohydrates in the biological systems is to be achieved, the issue of ease of obtaining the building blocks, development of new reaction methodologies and synthetic strategies have to be addressed. Even though a number of methodologies are reported in the literature, the subject still remains challenging as more and more new functions and needs for carbohydrates emerge from time to time. In line with the worldwide drive towards greener chemistry one of the areas the group focuses on is the development of catalytic and environmentally friendly reaction protocols for the transformation of glycals and 1,2-cyclopropanated sugars into useful derivatives. Glycals are C1-2 unsaturated sugar derivatives which have found wide application as building blocks in the synthesis of complex carbohydrate compounds. The research group has developed a number of simple and novel methods for the transformation of glycals and cyclopropanated sugars into 2-deoxy glycosides and suitably activated glycosyl donors. The methodologies so developed are being applied in the synthesis of medicinally valuable carbohydrate constructs of interest such as inhibitors of certain enzymes involved in the biosynthesis of the defensive mechanism of *mycobacterium* as well as development of HIV vaccine based on synthetic gp120 glycoconjugates. A number of metal complexes have been reported to posses anti-cancer and anti-HIV activity. However, the major drawback with most metal complexes is the associated toxicity to normal cells due to the toxicity of the ligands employed. To enhance the therapeutic activity of these complexes, use of non-toxic ligands such as carbohydrates has raised considerable interest. Thus, the other focus of this research group is to develop carbohydrate based metal complexes and nano-particles and study their Structure Activity Relationship (SAR) against TB, Malaria and HIV/Aids.

**Prof James Darkwa's** research centers around synthesis with special focus on applications in homogeneous catalysis and the development of metallodrugs. The group has developed several pyrazolyl ligand supported nickel complexes that are excellent ethylene oligomerization catalysts. It has recently been established that these nickel complexes act in tandem with ethyl aluminium dichloride to catalyse the oligomerization of ethylene to C4-C8 olefins. These olefins in turn alkylate toluene; a reaction that provides an efficient route to alkyl toluenes under very moderate conditions. The group has also developed several olefin polymerization catalysts using pyrazolyl ligands and chromium. The versatility of pyrazoles as nitrogen donor ligands in catalysts has made it possible to develop several catalysts for the production of biodegradable polymers from lactides and caprolactones, as well as for the co-polymerization of carbon monoxide with olefins. The catalysis work has three key collaborative partners outside South Africa. Dr Ilia Guzei at the University of Wisconsin has over the years been instrumental in structural and modeling work associated with the catalysts that have been developed. Professor Kyoko Nozaki at the University of Tokyo collaborates on the carbon monoxide and olefins co-polymerization project, while Dr Matt Clark at St Andrews University in Scotland is involved in hydrogenation catalysis that further extends the use of pyrazolyl metal complexes. In South Africa long term collaboration with Professor Selwyn Mapolie's group at Stellenbosch has proven very fruitful.

The initial use of pyrazoles in platinum and gold chemistry has led to a new interest in metallodrugs. Over the last 6 years several anti-cancer and anti-HIV agents have been identified, including a series of compounds for which a provisional patent as potential anti-cancer drugs has been filed. The success in developing metallodrugs was recently rewarded with two new projects on developing tandem metallodrugs, one supported by the Technology Innovation Agency (TIA) for HIV and TB, and another supported by Mintek's Nanotechnology Innovation Centre to convert metallodrugs into nanomaterials. The metallodrugs project is part of a long-term collaboration with Lund University in Sweden which has allowed several the postgraduate students in the group to visit this institution, the most recent being Ms Stacy Lillywhite who paid a research visit from October to December 2010. Ms Margaret Yankey is scheduled for a similar visit this year starting from the 1st of May to mid July.

Two other students in the group have had recent research visits to laboratories of our collaborative partners.

*Prof Darkwa and group*

*Prof Meijboom, Dr Muller and group*

From October to November last year Mr Collins Obuah worked on carbon monoxide co-polymerization catalysts at University of Tokyo. Currently Ms Letitia Benade is at St Andrews University in Scotland as the second UJ-St Andrews PhD student in Chemistry. Ms Benade's visit is supported by a commonwealth scholarship, which should allow her to spend another six months next year. Initial reports reaching the Department is that her research work is going on very well and that she is enjoying every minute of her stay in Scotland.

The research field of **Prof Gert Kruger** and **Mrs Charmaine Aderne** involves the experimental study of the crystal packing in the polymorphs of alkyl- and aryl-ammonium salts (mostly ammonium halides, nitrates, etc of long-chain alkanes and their derivatives) in order to establish the relative importance of hydrogen bonding and other intermolecular forces in directing molecular packing. They are currently investigating the structural phase transitions in the series of compounds containing the end-substituted alkane chain, $XC_nH_{2n}Y$, with n = 4 to 24 and X and Y = hydrogen, ammonium salts or similar structure directing groups. They examine the crystal structures and polymorphism in a series of compounds by thermo-analytical methods (DSC, TGA and hot stage microscopy) and diffraction techniques (powder and single crystal X-ray, neutron and electron diffraction). Organic compounds that contain linear methylene chains are economically and technically important as they include the synthetic and natural waxes, the polyethylenes, pharmaceuticals, fats and surfactants. Technological advances that will lead to improved industrial formulations will depend on a fundamental knowledge of the physical chemistry of their constituents and their interactions with emulsifiers. Polymorphism is the phenomenon in which the same chemical substance crystallizes in more than one crystal form. Modification of existing drugs by attachment of suitable alkanes may induce new packing arrangements resulting in novel and marketable products. The materials that they are studying present numerous academic challenges because the relationship between the crystal chemistry of such compounds and their (desirable) physical properties are not well understood. A study of the variation in the supramolecular interactions in crystals of long-chain compounds should provide further insights into the manipulation and exploitation of polymorph production.

**The meta-catalysis group** is lead by Prof Reinout Meijboom and Dr Fanie Muller. **Prof Reinout Meijboom** specialises in the design, synthesis and characterisation of dendritic macromolecules and organometallic dendrimers with novel reactivity and properties as well as the design, synthesis and characterisation of novel inorganic and organometallic compounds. Evaluation of catalytic activity of these compounds as homogeneous catalysts, immobilisation of homogeneous catalysts using dendrimers, biphasic systems, micro-emulsions, etc. and the evaluation of such systems is part of this work.


*Prof Gert Kruger and Mrs Aderne*

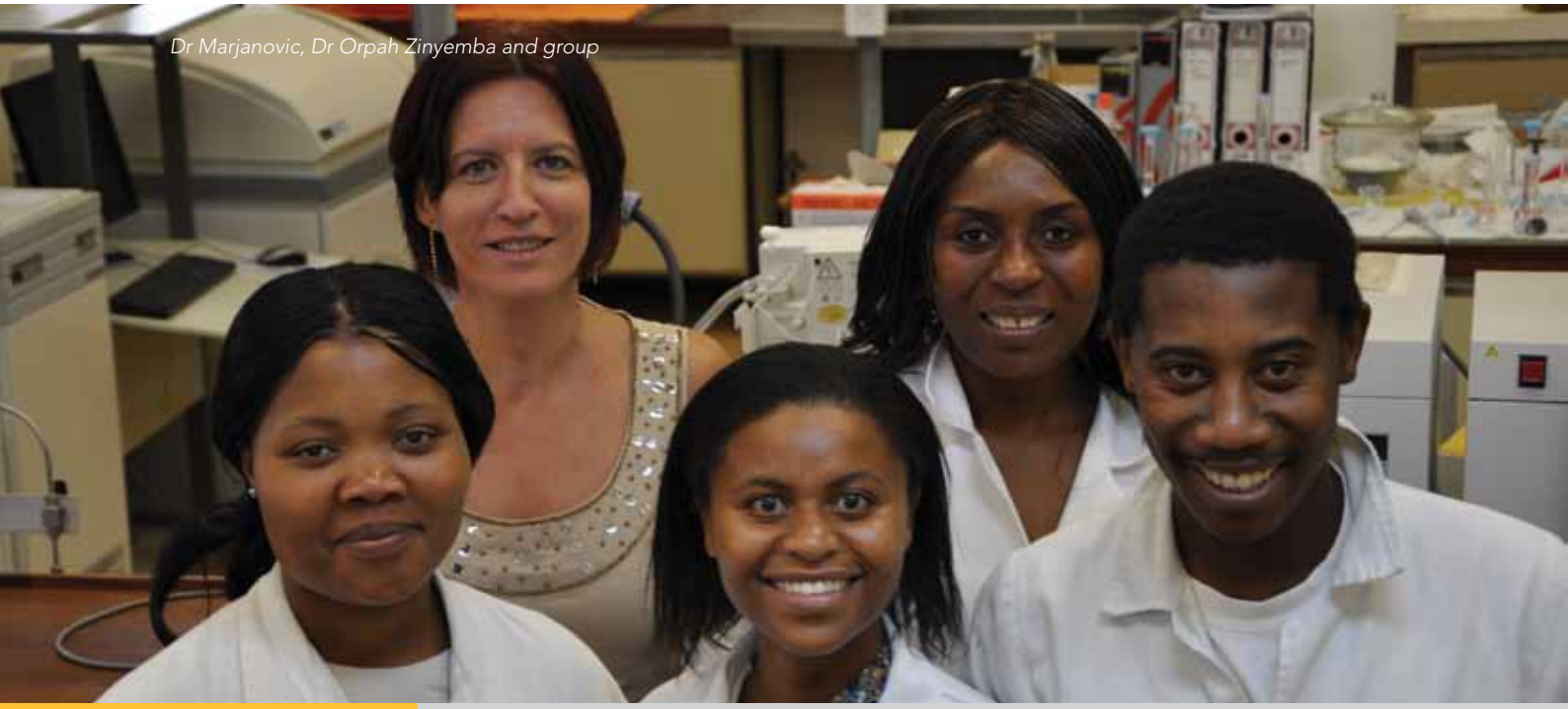
*Dr Laetitia den Drijven,*
*HOD from the Department of Chemistry*


*Prof Paul Coetzee*

He also has expertise in the synthesis and characterisation of air-sensitive compounds and the evaluation of coordination compounds using X-ray crystallography combined with spectroscopic methods. The research of **Dr Fanie Muller** focuses on crystallographic and computational aspects. Investigations into these two broad areas include packing disorders of organometallics compounds, steric and electronic behavior of group 15 ligands and small interactions of gold alloyed surfaces or nanoparticles. All of these have possible application in catalysis.

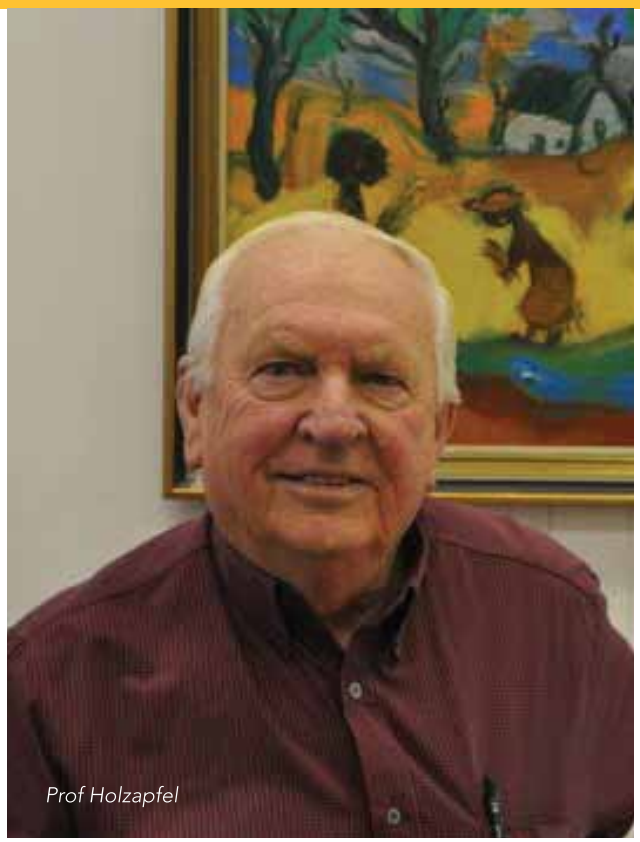
The **Analytical Chemists** are Prof Paul Coetzee, Dr Ljiljana Marjanovic and Dr Orpah Zinyemba. **Prof Paul Coetzee's** main area of research is the chemistry, analytical chemistry and speciation of trace elements.

He uses Atomic spectroscopy, AAS, ICP-OES, ICP-MS, X-ray fluorescence and HPLC in his studies on environmental pollution, sequential extraction, physical water treatment, defluoridation, authentication of agricultural products and provenance studies. **Dr Orpah Zinyemba** also is involved in research into environmental pollution and authentication of agricultural products using ICP-MS, AAS, ICP-OES and polarography. This includes the bio-sorption of heavy metals by micro-organisms. **Dr Ljiljana Marjonovic's** main area of research is Atomic Spectroscopy, specifically the use of slurry nebulisation techniques for the analysis of various samples by ICP-OES and ICP-MS. Another field of interest is the use of LA-ICP-MS as an analytical tool as well as for dating various minerals which is currently under development.



*Dr Marjanovic, Dr Orpah Zinyemba and group*

# Solid Gold
## Emeritus Professor


*Prof Holzapfel*

Should you happen to visit the Chemistry Department at UJ chances are that you will see a head of white hair bowed over a piece of paper shoulder to shoulder with a post-graduate student, while an animated discussion is underway, accompanied by many scribblings on said piece of paper. **Prof Cedric Holzapfel** is an Emeritus Professor in the Department and a well-respected mentor for students and staff alike. His career and the history of the Chemistry Department are interwoven to such an extent that it is difficult to separate the two.

Prof Holzapfel started his academic career at Stellenbosch University, where he obtained his BSc (1955) and MSc (1957) degrees with distinction. He then enrolled for a PhD at the University of Manchester and again graduated (1962) with distinction. On his return to South Africa he joined the CSIR as a researcher, but left in 1970 to take up an appointment as Professor of Chemistry at the then Rand Afrikaans University, a position he held until his retirement in 2002. When he started in the Department Prof Rein Arndt was the Chairperson and they were still housed on the Braamfontein Campus in the old Brewery buildings. The move to the current campus in Auckland Park happened during 1975 and the new facilities afforded the opportunity to accommodate more students. He was intensely involved in the teaching and training of both undergraduate and post-graduate students, acting as promoter for 35 MSc and 34 PhD students and publishing widely. His involvement also extended to numerous elements of the organisational and operational activities of the university. These included Chairman of the Department of Chemistry, Chairman of the Library Committee, Chairman of the Research Committee and Member of the Senate Executive Committee.

He held NRF research grants from 1984 to 2000 and held NRF ratings of A (1993) and A$^+$ (1998), a clear indication of his standing in the research community. In the period 1985 – 2002 Professor Holzapfel obtained private sector sponsorship for presenting Summer Schools of Chemistry presented by leaders of research from the U.S.A., U.K. and Europe. These schools were open and free of charge to graduates and staff of other universities and industry. Amongst other things these schools served to create awareness of the research interests and activities of the Department of Chemistry and played a vital role in the recruitment of post-graduate students.

He was directly involved with the activities of the South African Chemical Institute (1980 – 2000), amongst others as member of the editorial board and assistant editor of the South African Journal of Chemistry. He was also responsible (as a member of organising committees) for the organising of numerous national and international (e.g. IUPAC, Heterocyclic Chemical Society, Homogenous Catalysis Society) conferences. This also contributed to elevating the profile of the Institution as well as of the Department of Chemistry in the International arena.

Prof Holzapfel had formal associations with SASOL (1997 – 2008), AECI (1990 – 1998) and the CSIR (1995 – 2005) as Chemistry Advisor. He has played a vital part in furthering collaboration between the Department of Chemistry and various Industry partners, the obtaining of research grants and grants for upgrading of scientific equipment. Since his retirement as full professor (2002) he continued to be involved with teaching and research at all levels at the request of the Department of Chemistry.

From the above it is clear that Professor Holzapfel played a vital part in the establishment of the Department of Chemistry and the Institution as noteworthy players in the National and International field of Chemistry. He is still held in the highest regard by peers and ex-students alike and is consulted on a daily basis by both industrial companies and confused post-graduate students. He has made an invaluable contribution to the Chemical Industry in this country by delivering excellent synthetic organic chemists who currently form the core of many Research and Development groups as well as of the management of various companies, are involved in the stock exchange, are top academics, the list goes on and on. He has recently been awarded the M.T. Steyn Medal for Scientific and Technological Achievement by the South African Academy for Science and Art for his lifetime contribution to the Sciences. It is one of the most important honours of the Academy for leadership at the highest level in the areas of Science and Technology and can only be awarded to a person once. It is a privilege to still have him associated with the Department of Chemistry and to be able to benefit from his wisdom.

# Research Academy
## for Undergraduates in Chemistry

In 2009 **Prof Reinout Meijboom** proposed the establishment of a research academy for undergraduate students in Chemistry. The aim of the project was to provide undergraduate students with research exposure in order to transfer knowledge of best practice in chemistry (i.e. *learning* to become a chemist) and to prepare them for the post-graduate experience. Experimental experience as well as excitement about research can be provided through this project, while a stable, empowering environment is generated to enable students to excel in their studies and to continue with post-graduate studies. A pilot study conducted over the last two years was very successful and the Department is now ready to implement the Academy fully.

## Problem identification

A number of problems exist in our society that prevents the best-possible education for our students, especially in a subject like chemistry where research is experimentally driven. Some of the areas we are trying to address by using undergraduate students to do research are:

- Additional experimental training for students.

The current experimental training in chemistry is not adequately preparing the students for a research experience due to time constraints. By enrolling undergraduate students in research projects, additional experimental training can take place.

- Ensuring that students are engaged with their study full-time.

Removal of several distracting factors (both financial and social) and replacing them with empowering factors that support the student's studies increases chances of success in their studies.

- Removal of social pressures to stop studies.

Most of our undergraduates are first-generation university students. The social environment (parents, friends) does not realize what a university degree entails, and sees it as 'school'. Our students

experience tremendous pressures from their home environment to 'stop going to school and start working'. By providing these students work that is (intellectually) supporting their studies, they are able to negotiate these pressures.

## Rationale and motivation

We see research as a means to further develop our profile in our demonstrated areas of interest - chemistry being one discipline where UJ has already demonstrated its ability to generate local profile. In order to be recognized as a *centre of excellence* in sciences, it is necessary to provide additional training experience to undergraduate students. An undergraduate research program will not only distinguish us from the rest of the educational and research market, but will also build on our strengths. The program will improve skills development as well as the attitude and knowledge of the students involved.

A large number of students find it financially necessary to work a job in their spare time, which typically does not provide them with experience in the area they are studying. It would benefit these students tremendously if they were given an opportunity to participate in research, rather than work as waiters, not only from a skills development point of view but also from a CV building point of view. A job as researcher on campus takes place in a secure, safe and well-known environment. The experience gained will clearly distinguish UJ graduates from those of other universities in South Africa. Additionally, early exposure to research – as well as being treated like researchers – motivates students to enrol for post-graduate studies. Since the number of post-graduate students in chemistry is declining nationwide, this is of critical importance to the future growth of the Chemistry Department.

## Modus Operandi

Undergraduate students (second year BSc) are employed as temporary researchers in the Department of Chemistry. These students are expected to treat their research project as a job and are being paid and treated accordingly. Predetermined hours, so as not to interfere with their studies, are agreed on so they work at expected times. The projects allocated to these students are of a sufficiently (experimentally) simple nature to enable them to generate enough results for a publication (if necessary several of these projects can be combined to form a larger publication). This exposes the students to a research environment, as well as offering first-hand experience with the various tools necessary for chemistry research.

As can be expected, a lot of time is needed to teach/supervise these students. Various post-graduate students, post-doctoral fellows and previous year's students act as *role models*. Additional to the necessary motivation these role models provide, a lot of personal attention can thus be dedicated to the students, which facilitates learning on their side. All in all, this creates a *home away from home* for the undergraduates, as well as a readily available knowledge pool that can be used when a student is struggling with a certain subject.

## Outputs

We ran a pilot study on a limited number of students during the past year and a half. Four third year students were enrolled in the research program in 2009. Of these students, three did their BSc Hons degree and were the top three of their class. All three are currently enrolled for a MSc degree. The fourth student has decided to continue his career in chemical engineering and is enrolled for a BSc Hons degree in chemical engineering. Two publications have been published in ISI accredited journals from students work and a third one has been submitted.

# Research Centre for Synthesis and Catalysis

The Department of Chemistry is proud to be the home of a research centre of the University. It has been instituted to drive innovative research that focuses on synthesis and catalysis with a view to investigating areas of interest to the South African and broader chemical industries. The goals of the Centre can be summarised as follows:

1. To train post-graduate students at honours, masters and doctoral levels.
2. To conduct and publish fundamental and applied research in the disciplines of synthesis and catalysis.
3. To develop novel chemistry technologies and methodologies.
4. To develop and maintain laboratory and capital infrastructure appropriate to the focus of the Centre.
5. To develop procedures for incorporating Centre activities in the undergraduate and honours level lectures.
6. Carry out community outreach programmes within the general ambit of chemistry and the Centre's research programme.

The centre has thus far been extremely successful in achieving all its goals and will continue to grow in future.

# Chemistry in the limelight

**Professor Bradley Williams**, who specialises in synthesis and catalysis, recently had two of his articles singled out as being in the **top ten most read articles** in two highly rated journals, namely: *Drying of organic solvents: quantitative evaluation of the efficiency of several desiccants, DBG Williams, M Lawton, 2010, J Org Chem 2010, 75, 8351 (front cover art for issue 24, Dec 2010. (IF 4.2))* and *Mild water-promoted selective deacetalisation of acyclic acetals, DBG Williams, A Cullen, A Fourie, H Henning, M Lawton, W Mommsen, P Nangu, J Parker, A Renison, Green Chem. 2010, 12, 1919).* This journal has an impact factor of 5.8. Prof Williams also has two students who received prizes. **Mrs Alicia Renison** was awarded the James Moir Medal for the best Chemistry student in the honours group (2009) and also received a prize from the South African Academy for Science and Art for the best presentation for an MSc student at the annual student symposium. **Mr Sandile Simelane,** a PhD student with Prof Williams, has been awarded the S2A3 prize for the best MSc thesis in the Faculty.

The Raikes Medal of the South African Chemical Institute for 2009 was awarded to **Prof Reinout Meijboom.** The award is made to a person, under the age of 40 on 31 December proceeding the year of the award, whose original chemical research shows outstanding promise, as judged by the person's publications in reputable journals. It is further stipulated that the research shall have been performed in South Africa. He also received the Faculty of Science's award for the top achiever in 2010 in the category Senior lecturer/Lecturer.

A PhD student of Prof Meijboom, Nathan Anthonels, was awarded the Prize as the best PhD presenter at the 2010 SACI Young Scientist Symposium.

One of Prof Darkwa's PhD students, **Ms L Benade**, is currently at St Andrews University in Scotland as part of the exchange programme between UJ and St Andrews. She will spend 6 months there, returning to South Africa in July and may return for another six months. At the end of her studies she will receive a joint PhD from the two institutions.

*Mrs Alicia Renison*

*Mr Nathan Anthonels*

*Mr Sandile Simelane*

*Ms Letitia Benade*


# Next Issues

**This Newsletter focusses on Chemistry and the next Newsletter on Chemical Technology. Thereafter it will be:**

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|---|---|
| **MAY** | Geology \| Geography, Environmental Management and Energy Studies |
| **JUNE** | IT \| Applied Mathematics \| Statistics \| Mathematics |
| **AUGUST** | Biochemistry \| Zoology \| Botany \| Food Technology \| Biotechnology |
| **SEPTEMBER** | Physics |


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