



**CENTRE OF THEORETICAL CHEMISTRY AND PHYSICS (CTCP)  
INSTITUTE OF FUNDAMENTAL SCIENCES**

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## **CTCP ANNUAL REPORT 2005**

### **Personnel**

Prof. Peter Schwerdtfeger

Dr. Robert P. Krawczyk (Research Officer)

### **Honorary Research Fellows**

Dr Tilo Söhnel (Senior Lecturer, Auckland University)

### **Marsden Postdoctoral Fellow**

Dr Matthias Lein

### **PhD Students**

Behnam Assadollahzadeh

Susan Biering

Nicola Gaston

Andreas Hermann

Ivan Lim

Christian Thierfelder

Brian Vest

### **Exchange Students**

Daniel Benker (LMU Munich)

Christian Olendrowitz (TU Berlin)

Philipp Mörschel (Philipps Universität Marburg)

## **GENERAL COMMENTS**

2005 was a very successful year for the TCP centre as the number of publications increased substantially compared to the year before. The main reason was that the double-helix was up and running and all software compiled and installed. It also saw three new PhD students joining. 2005 was the second year of a Marsden grant running, worth NZ\$ 630,000 over three years. The TCP group has solved a long-standing problem raised by Max Born in 1930 concerning the packing of rare gas atoms (fcc vs. hcp), which is in press in Phys. Rev. B (19 pages!). We believe that this paper will become a classic. We note invitations to a number of international conferences and the election of the TCP director to chair the next NZIC conference in Rotorua in December 2006, and to organize a symposium on "Relativistic,

quantum electrodynamic and electroweak effects in atoms and molecules” in Chania (Greece) in October 2006. All the main players in this field accepted the invitation to participate.

There was also some lesser good news. The CTCP’s Marsden grant on “parity violation in molecules” was rejected in the final round by the PSE panel despite very clear “outstandings” from the two referees. To our opinion this is our most important research project for the future. The message received from the chairperson of the Marsden panel was that outstanding reports do not automatically imply that the research project is to be funded. This raises serious questions on how Marsden applications are assessed. Another concern is that at Albany space becomes now very tight and a larger building is needed for chemistry and physics. Our secretary is far away from us in another building and we do not have space for accommodating her in either building 40 or 44. Furthermore, more postgraduate students are needed (note that IFS at Albany currently does not attract postgraduate students from PN), and new research equipment is urgently required (upgrade of the double-helix). Two buildings need air-conditioning as the working environment in summer becomes unbearable in the huts occupied, and we experienced a number of failures of our desktop computers and work-stations due to high temperature. This is due to the fact that our computers are constantly running software applications. The failure of the Albany appointee (Gero Schmidt) to fulfil responsibilities is also noted. Recruitment will continue to strengthen theoretical physics research at Albany. It has however been very difficult to attract the top-listed candidates to Albany. The lack of an appropriate research infrastructure for science and office space in Albany is seen as the major reason for this.

Invitations to a number of conferences were received and some accepted (see below). We saw two PhD completions: Ivan Lim, who received a postdoctoral fellowship at KAIST in Korea, and Nicola Gaston, who received a research fellowship at the Max-Planck Institute for the Physics of Complex Systems in Dresden (Germany). The CTCP was host for a Workshop on “The Chemistry and Physics of Heavy and Superheavy Elements” at Massey University (Albany), sponsored by the New Zealand Ministry of Research, Science and Technology and the Deutsche Forschungsgemeinschaft (DFG) Programme, and organized by the Director of CTCP and Prof. Burkhard Fricke (Kassel). More than a dozen international eminent scientists participated in this workshop, together with members from Massey and Auckland University. A conference proceeding was published, and a similar second workshop is planned in near future to take place in Germany. We also had a number of international visitors (see below) and will continue to host a large number of researchers from overseas.

For 2006 plans are going ahead for further appointments in the area of theoretical sciences and to prepare for a CoRE proposal for 2007/8. We will see the arrival of Dr. Patrick Bowman working in the area of theoretical nuclear physics, and hopefully Dr. Joachim Brandt in the area of solid state physics. Building number 40 at Oteha Rohe will be the new theoretical physics building.

## **NOTABLE DEVELOPMENTS**

### **Double-Helix Supercomputer**

Massey University took delivery of its new Double Helix Cluster Computer end of 2004 with up to ten times the computational power of the university's existing supercomputer, the 64-node Helix 1. Whereas the Helix 1 cluster, commissioned about four years ago, consists of 32-bit computers in normal PC cases, the 64-bit Double Helix is mounted in a 19" rack, and takes up less than a tenth of the space of the old setup. Insite Technology in Christchurch built the cluster for Massey University, worth about \$300,000 including the gigabit ethernet network used to connect the 19 slave nodes with the master node with a managed Cisco switch. The nodes are equipped with dual AMD Opteron 250 processors that run at 2.4 GHz

and have 1 MB of L2 cache each. The Opteron 250 also uses AMD's HyperTransport bus, running at 800MHz. Each slave node has 4GB of RAM, with the master controlling node having 16GB RAM. Insite mounted all of that plus dual 120GB IDE hard drives on a Rioworks HDAMA server motherboard, and squeezed the lot into 1U 19" Chenbro RM311 chassis.

The Double Helix runs the open source Rocks Cluster Linux distribution. The OS and new set-up is considerably easier to manage than the old one — changes only need to be made to the Master Node, from which they are then automatically propagated to the Slave Nodes. The extra computational power will be welcome for its student and researchers in the areas of bioinformatics and computational chemistry and physics. Users of the existing Helix 1 cluster are currently experiencing long queues during busy times, sometimes up to 19 days. The Double Helix enable Massey's researchers to participate in overseas projects where its academic counterparts already enjoy access to high-power super computer clusters.

After months of software development and maintenance carried out by Robert Krawczyk and Matthias Lein with the assistance of Stephen Ford (IIMS) the Double-Helix was ready for production work by March 2005. It has already proven to be a very stable machine with nodes rarely going down. We experience no difficulties in running parallel jobs in contrast to the older helix computer which runs in an unstable software environment. See also Massey news: [http://masseynews.massey.ac.nz/2004/Press\\_Releases/28\\_24\\_04.html](http://masseynews.massey.ac.nz/2004/Press_Releases/28_24_04.html)

The double-helix supercomputer at Albany is hopefully being upgraded in 2006. We aim for 12 8-way dual core AMD machines at a total cost of ca. 700,000 NZ\$.

### **Major Grants Received/Continuing**

Marsden Fund (2003-06)

Principle Investigator: P. Schwerdtfeger

NZ\$ 210,000 per annum

Title: *Nanostructures of Gold – From Low-Dimensional Assemblies to Heterogeneous Catalysis*

The New Zealand Ministry of Research, Science and Technology and the Deutsche Forschungsgemeinschaft (DFG) Programme

Organizer: P. Schwerdtfeger

NZ\$ 24,000

Title: *The Chemistry and Physics of Heavy and Superheavy Elements*

Albany Strategic Fund / Massey University

Title: *Physics and Chemistry of Excited Systems: Photodynamics and Large Scale Numerical Simulations.*

Principle Investigator: R. P. Krawczyk

NZ\$ 15,000

Behnam Assadollahzadeh and Nicola Gaston received funding from IFS to attend the Asian-Pacific Conference on Theoretical Chemistry in Bangkok, May 2-6.

### **Visitors**

Prof. Tom Ziegler (Department of Chemistry, University of Calgary)

Prof. Dietmar Kolb (Department of Physics, University of Kassel)

Prof. Keiji Morokuma (Department of Chemistry, Emory University, USA)

Dr. Patricia Hunt (Imperial College, London)

## Seminars

P. Schwerdtfeger gave a number of talks at Massey University (3 in Albany and 2 in Palmerston North). He also gave invited talks at universities in Otago, Frankfurt, Stuttgart and Darmstadt. M. Lein gave various seminars in Albany, Stuttgart and Marburg. R. Krawczyk gave seminars in Albany.

## Teaching

In 2005 we saw the arrival of Mrs. Stephanie Wayper (Tutor) at Albany. She did an outstanding job in teaching stage 1 physics and organizing all the stage 1 and 2 laboratory classes. P. Schwerdtfeger taught a postgraduate course on Theoretical Chemistry in Palmerston North. All members of the CTPC were involved in chemistry and physics lab teaching. P. Schwerdtfeger taught three weeks of thermodynamics in stage 1 physics. Behnam Assadollahzadeh was involved in tutorials and student supervision. Teaching commitments will increase with the start of postgraduate degrees in chemical physics and in mathematical physics in 2007.

## PhD Theses

*Behnam Assadollahzadeh* (PhD thesis): *Properties of metal clusters of Au, Cs and Sn.*  
Supervisor: P. Schwerdtfeger.

*Susan Biehring* (PhD thesis): *Relativistic structure changes in group 12 oxides.*  
Supervisor: P. Schwerdtfeger.

*Nicola Gaston* (PhD thesis): *Mercury Clusters – from van der Waals molecules to the metallic solid.*  
Supervisor: P. Schwerdtfeger. Completed July 2005.

*Andreas Hermann* (PhD thesis): *Adsorption properties of water surfaces.*  
Supervisor: P. Schwerdtfeger.

*Ivan Lim* (PhD thesis): *Static Electric Dipole Polarizabilities of Atoms and Molecules.*  
Supervisor: P. Schwerdtfeger. Completed April 2005.

*Christian Thierfelder* (PhD thesis): *Applications to the Dirac equation – from relativistic effects to electroweak interactions.*  
Supervisor: P. Schwerdtfeger.

*Brian Vest* (PhD thesis): *Nucleation of chromium dihalides – from the gas phase to the solid state.* Supervisor: P. Schwerdtfeger.

## Lectures at Conferences / Meetings

Given by *P. Schwerdtfeger*

- 2nd Asian Pacific Conference on Theoretical & Computational Chemistry (APACTC), Bangkok (May 2-6): *The Search for Parity Violation Effects in Chiral Molecules*  
Also served as Session Chair
- 1<sup>st</sup> New Zealand/German workshop on heavy and superheavy element chemistry and physics, Massey University, Albany (May 28-29)  
*The performance of density functional theory for electric field gradients*, in *The Chemistry and Physics of Heavy and Superheavy Elements*
- Joint New Zealand / Australian Alexander von Humboldt Meeting, Brisbane (September 2-5) *Biomolecular Homochirality*  
Also served as Session Chair
- 19<sup>th</sup> Colloquium on High Resolution Molecular Spectroscopy, Salamanca (11-16 September)  
*The Search for Parity Violation Effects in Chiral Molecules*
- International Conference of Computational Methods in Sciences and Engineering (ICCMSE), Loutraki, Greece (October 21-26)  
Two invited talks: a) *Polarisabilities of Mercury Clusters*; b) *The Search for Absolute Chirality*.  
Also served as Session Chair

- PACIFICHEM Meeting in Hawaii (December 15-20)  
Two invited talks: a) *The Chemistry of Superheavy Elements*; b) *An old problem solved: The packing of rare gases*.  
Also served as Session Chair
- Waikato – Auckland – Massey Inorganic Chemistry Symposium, University of Waikato (May 2005)  
*The packing of rare gases*.

Given by *M. Lein*

- 2nd Asian Pacific Conference on Theoretical & Computational Chemistry (APACTC), Bangkok (May 2-6): *The Chemical Bond in the Light of an Energy Decomposition Analysis. Why do the Heavy-Atom Analogues of Acetylene  $E_2H_2$  ( $E = Si - Pb$ ) Exhibit Unusual Structures?*
- 1<sup>st</sup> New Zealand/German workshop on heavy and superheavy element chemistry and physics, Massey University, Albany (May 28-29)  
*Catalytic Activity of Au(III)*
- Waikato – Auckland – Massey Inorganic Chemistry Symposium, University of Waikato (May 2005)  
*Catalytic Activity of Au(III)*

Given by *N. Gaston*

- 1<sup>st</sup> New Zealand/German workshop on heavy and superheavy element chemistry and physics, Massey University, Albany (May 28-29)  
*The frequency dependent dipole-polarizability of the mercury dimer*

Given by *R. P. Krawczyk*

- 2nd Asian Pacific Conference on Theoretical & Computational Chemistry

*(APACTC), Bangkok (May 2-6): Coinage Metal Halide Oligomers*

- 1<sup>st</sup> New Zealand/German workshop on heavy and superheavy element chemistry and physics, Massey University, Albany (May 28-29)  
*Coinage Metal Halide Oligomers*

Given by *T. Söhnel*

- 2nd Asian Pacific Conference on Theoretical & Computational Chemistry (APACTC), Bangkok (May 2-6): *Solid State Density Functional Calculations of Halides and Oxides*
- 1<sup>st</sup> New Zealand/German workshop on heavy and superheavy element chemistry and physics, Massey University, Albany (May 28-29)  
*Fe, Ru and Ir containing tin cluster compounds*
- Waikato – Auckland – Massey Inorganic Chemistry Symposium, University of Waikato (May 2005)  
*New exciting solid state compounds*
- Joint New Zealand / Australian Alexander von Humboldt Meeting, Brisbane (September 2-5) *New exciting solid state compounds*

Given by Behnam Assadollahzadeh

- 1<sup>st</sup> New Zealand/German workshop on heavy and superheavy element chemistry and physics, Massey University, Albany (May 28-29)  
*Density functional study of structural and physical properties of gold and cesium clusters.*

### **Posters**

- Nicola Gaston, 2nd Asian Pacific Conference on Theoretical & Computational Chemistry (APACTC), Bangkok (May 2-6): *Many-body effects in mercury clusters.*
- Behnam Assadollahzadeh, 2nd Asian Pacific Conference on Theoretical & Computational Chemistry (APACTC), Bangkok (May 2-6): *Density functional study of structural and physical properties of gold clusters.*

### **Administrative Duties**

P. Schwerdtfeger was chair of the IFS Research and Equipment Committee, the NZIC conference committee, and member of the IFS Management Committee and the Albany Academic Committee. He also serves as the President of the New Zealand Alexander von Humboldt Association and is on the board of the Asian Pacific Theoretical & Computational Chemistry Society. He is also on the editorial board of Journal of Computational Chemistry, Structural Chemistry and Lecture Series on Computer and Computational Sciences. R. Krawczyk attended a meeting “German Language in New Zealand” organized by the German Embassy in Wellington. P. Schwerdtfeger and R. Krawczyk are also members of the high-performance computer committee.

### **Conferences Organizations**

The theoretical chemistry centre at Albany hosted a joint New Zealand/German workshop on superheavy element chemistry, which was well received.

Invitations accepted to be the chairperson of the next NZIC meeting in Rotorua, December 2-6, and to organize a symposium on “Relativistic, Quantum electrodynamic and electroweak

effects in atoms and molecules” in Chania (Greece) in October 2006.

## Other work

Papers refereed: P. Schwerdtfeger refereed 53 papers from international journals including Physics Letters A, J. Phys. Chem. A, Angewandte Chem. Int. Ed., Chemistry-A Europ. J., PCCP, Chem. Phys. Lett., J. Comput. Chem., J. Org. Chem., J. Chem. Phys., Europ. J. Inorg. Chem., Inorg. Chem., Phys. Rev. Lett., Theoret. Chem. Acc., J. R. Soc. NZ, J. Agricult. Food Chem., Aust. J. Chem., J. Mol. Struct. (Theochem.)

### *PhD and MSc theses refereed:*

MSC thesis from Auckland University: “Identification of the Pigments, Fatty Acids and Glycogen Present in the Gonads of Cultured Sea Urchins” by Qiong Chen. (Supervisor Charmian O’Connor)

PhD thesis from Otago University: (Supervisor Henrik Kjaergaard)

## PUBLISHED WORK

### Papers published in refereed journals

- M. Lein, A. Krapp, G. Frenking, “Why do the Heavy-Atom Analogues of Acetylene  $E_2H_2$  ( $E = Si - Pb$ ) Exhibit Unusual Structures?” *J. Am. Chem. Soc.* **127**, 6290-6299 (2005).
- T. Söhnel, H. Hermann, P. Schwerdtfeger, “Solid State Density Functional Calculations for the Group 11 Monohalides”, *J. Phys. Chem. B* **109**, 526-531 (2005).
- P. Schwerdtfeger, T. Saue, J. N. P. van Stralen, L. Visscher, “Relativistic Second-Order Many-Body and Density Functional Theory for the Parity-Violation Contribution to the C-F Stretching Mode in  $CHFCIBr$ .”, *Phys. Rev. A* **71**, 012103-1-7 (2005).
- J. Anton, B. Fricke, P. Schwerdtfeger, “Non-collinear and collinear four-component relativistic molecular density functional calculations”, *Chem. Phys.* **311**, 97-103 (2005).
- I. S. Lim, P. Schwerdtfeger, B. Metz, H. Stoll, “Relativistic Small-Core Energy-Consistent Pseudopotentials for the Group 1 Elements from K to Element 119”, *J. Chem. Phys.* **122**, 104103-1-12 (2005).
- P. Schwerdtfeger, R. Bast, M. C. L. Gerry, C. R. Jacob, M. Jansen, V. Kellö, A. V. Mudring, A. J. Sadlej, T. Saue, T. Söhnel, F. E. Wagner, “The quadrupole moment of the  $3/2^+$  nuclear ground state of  $^{197}Au$  from electric field gradient relativistic coupled cluster and density functional theory of small molecules and the solid state.” *J. Chem. Phys.* **122**, 124317-1-9 (2005).
- I. S. Lim, P. Schwerdtfeger, T. Söhnel, H. Stoll, “Ground-State Properties and Static Dipole Polarizabilities of the Alkali Dimers from  $K_2^n$  to  $Fr_2^n$  ( $n=0, +1$ ) from Scalar Relativistic Pseudopotential Coupled Cluster and Density Functional Studies”, *J. Chem. Phys.* **122**, 134307-1-7 (2005).
- M. A. Bennett, S. K. Bhargava, J. F. Boas, R. T. Boéré, A. M. Bond, A. J. Edwards, Si-Xuan Guo, A. Hammerl, J. R. Pilbrow, S. H. Privér, P. Schwerdtfeger, “Electrochemically Directed Synthesis and Characterization of a Novel  $[Pt_2(\mu-\eta^1, \eta^1-C_6H_3-5-Me-2-AsPh_2)_4]^+$  Lantern Complex that Contains a Pt-Pt Bond Order of 0.5”, *Inorg. Chem.* **44**, 2472-2482 (2005).
- A. J. Nielson, C. Shen, P. Schwerdtfeger, J. M. Waters, “Synthesis, Structure, Coordination Expansion and Theoretical Modelling of Ti(IV) Dichloro-bisphenoxide Complexes”, *Europ. J. Inorg. Chem.* 1343-1352 (2005).

J. Crassous, Ch. Chardonnet, T. Saue, P. Schwerdtfeger, ‘Recent experimental and theoretical developments towards the observation of parity violation (PV) effects in molecules by spectroscopy’, *Org. Biomol. Chem.* **3**, 2218-2224 (2005).

### **Book chapters**

R. Tonner and P. Schwerdtfeger, “Density Functional Calculations for Static Dipole Interaction Polarizabilities of Ne<sub>N</sub> Cluster up to  $N < 30$ .” *In the Frontiers of Computational Science*, in *Lecture Series on Computer and Computational Sciences*, eds. G. Maroulis, T. Simos, Volume 3, Brill Academic Publishers, Leiden, The Netherlands, 2005, pp. 223-228.

### **Books**

M. Lein and P. Schwerdtfeger (ed.), “The Chemistry and Physics of Heavy and Superheavy Elements,” Proceedings of the First German / New Zealand Workshop on Heavy and Superheavy Elements, Massey University Press, Palmerston North (2005); ISBN 0-473-10027-4. 192 pages.

### **Conference Proceedings**

M. Lein, “Catalytic Activity of Au(III)”, in “The Chemistry and Physics of Heavy and Superheavy Elements,” Massey University Press, Palmerston North (2005); pgs. 39-42.

N. Gaston, “The frequency dependent dipole-polarizability of the mercury dimer”, in “The Chemistry and Physics of Heavy and Superheavy Elements,” Massey University Press, Palmerston North (2005); pgs. 95-102.

B. Assadollahzadeh, “Density functional study of structural and physical properties of gold and cesium clusters”. in “The Chemistry and Physics of Heavy and Superheavy Elements,” Massey University Press, Palmerston North (2005); pg. 43-51.

R. Krawczyk, “Coinage Metal Halide Oligomers”, in “The Chemistry and Physics of Heavy and Superheavy Elements,” Massey University Press, Palmerston North (2005); pg. 135-143.

T. Söhnle, “Fe, Ru and Ir containing tin cluster compounds”, in “The Chemistry and Physics of Heavy and Superheavy Elements,” Massey University Press, Palmerston North (2005); pg. 135-143.

P. Schwerdtfeger, “The performance of density functional theory for electric field gradients”, in “The Chemistry and Physics of Heavy and Superheavy Elements,” Massey University Press, Palmerston North (2005); pg. 185-192.

Prof. Peter Schwerdtfeger  
**Date:** March 9, 2007