CENTRE OF THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
INSTITUTE OF FUNDAMENTAL SCIENCES
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CTCP ANNUAL PERFORMANCE REPORT 2006

Activities and achievements: 2006 was again a very successful year for our CTCP. Two new academic staff arrived to join the physics section. We also saw the arrival of three new PhD students and one research fellow. We hosted a number of international visitors. The double-helix computer ran without major down-time for the whole year. In fact, the machine is 100% over-committed (usage could be twice as high) with 0% idle time. All standard software is now installed and running. As a consequence, the number of publications increased substantially compared to the year before. However, with the arrival of new staff new research equipment is urgently required (upgrade of the double-helix).

2006 was the third year of a Marsden grant running, worth NZ$ 630,000 over three years. In addition, we had another Marsden grant approved (the third largest in the country, and the largest at Massey University). This grant on "parity violation in molecules" is to our opinion our most important research project for the next three years and involves extensive collaboration with three research groups in France (Strasbourg, Rennes and Paris) and one in Amsterdam.

The theoretical chemistry group has solved a long-standing problem raised by Max Born in 1930 concerning the packing of rare gas atoms (fcc vs. hcp), which appeared in Phys. Rev. B (19 pages!). We believe that this paper will become a classic in the field of solid-state physics. We note invitations to a number of international conferences and the election of the CTCP director (PS) to chair the NZIC conference, which was held in Rotorua in December 2006. We received comments that the conference was the best NZIC conference held so far. Each plenary speaker was of Nobel prize quality (two already received the Wolf prize). PS was also invited to organize a symposium on "Relativistic, quantum electrodynamic and electroweak effects in atoms and molecules", held in Chania (Greece) in October 2006. All the "main players" in this field accepted the invitation to participate.

Invitations to a number of conferences for 2007 were received and some already accepted. One of our former PhD students, Dr. Nicola Gaston, received the ICCMSE Young Scientist Excellence Award for 2006 based on her research carried out at Massey University.

Our secretary (Vesna Davidovic-Alexander) moved to building 44, and an additional postgraduate office space has been created in building 40. Building 40 at Oteha Rohe is now the new theoretical physics building.

Other activities: 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, and the Council of the Royal Society of New Zealand. He is also on the editorial board of Journal of Computational Chemistry, Structural Chemistry and Lecture Series on Computer and Computational Sciences. He also served on the review panel of the Otago University Chemistry Department. J. Brand served on the IFS Research and Equipment Committee.

P. Schwerdtfeger was the chairperson of the NZIC2006 conference in Rotorua, December 2-6. He also organized a symposium on “Relativistic, Quantum electrodynamic and electroweak effects in atoms and molecules” in Chania (Greece) in October 2006.
M. Lein was a member of the organizing committee of the NZIC Meeting 2006 “Back to the basics”. J. Brand served on the organizing committee of the international conference “SOLIQUANTUM'06: Solitons and nonlinear phenomena in degenerate quantum gases” at the Universidad de Castilla-la Mancha in Cuenca, Spain (Sept. 27-30). The conference was well received by the 54 international participants.
All members of CTPC were involved in chemistry and physics lab teaching. P. Schwerdtfeger taught a postgraduate course on *Theoretical Chemistry* (in Albany); three weeks of *Thermodynamics* for year 1 physics, and three weeks (together with M. Lein) of *Introduction to Quantum Theory* for the year 3 Materials course. P. Bowman taught stage 2 digital electronics. M. Lein was involved in lab-teaching at the stage 1 level in Chemistry. He also held three lectures in Peter Schwerdtfeger's lecture course on *Introduction to Quantum Theory* in Palmerston North. 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 2008.
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. 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 which is not an ideal situation for our research performance.

Future opportunities and directions: The double-helix supercomputer at Albany is hopefully being upgraded in 2007. We aim for 12 8-way dual core AMD machines at a total cost of ca. 700,000 NZ$. Another possibility being discussed is to join the supercomputer project of Canterbury University. Either option is fine for us. Just to mention that the QCD group at Adelaide has just bought a similar machine to the one we want, but about twice as big.
Two buildings need air-conditioning as the working environment in summer becomes unbearable in the huts occupied. Again we experienced a number of failures of our desktop computers and work-stations due to high temperatures. This is due to the fact that our computers are constantly running software applications. A possible move into the IIMS building is currently being discussed.
One Marsden grant was received starting February 2007 and the main focus of the theoretical chemistry group will be on parity violation effects in molecules.

Performance against objectives: All objectives were met as we are a very productive research centre with an outstanding performances at the international level. All papers published are in highly acclaimed journals. One Marsden, one ISAT and one Dumont D’Urville grant received for 2007.

Appendix

Personnel
Prof. Peter Schwerdtfeger (Director of CTCP, Deputy Director of IFS)
Dr. Joachim Brand (Senior Lecturer, Deputy Director of CTCP)
Dr. Patrick Bowman (Lecturer)
Dr. Robert P. Krawczyk (Research Officer, until June 26)
Dr. Matthias Lein (Research Officer , from August 24)

Honorary Research Fellows
Dr. Tilo Söhnel (Senior Lecturer, Auckland University)

Postdoctoral Fellows
Dr. Matthias Lein (Marsden fellow, until August 23)
Dr Gloria E. Moyano (Marsden fellow, from September 1 to October 31)
Elke Pahl (from July 1)

PhD Students
Behnam Assadollahzadeh
Susan Biering
Andreas Hermann
Christian Thierfelder
Brian Vest

Exchange Students
Sacha Schäfer (TU Darmstadt)

Secretary
Vesna Davidovic-Alexander

Visitors
Long Term:
Prof. Dietmar Kolb (University of Kassel, Germany, November 2006-April 2007)
Prof. Ian Hamilton (Wilfried Laurier University, Canada, December 2006 – June 2007)
Dr. Alexander Yu. Cherny (Bogoliubov Laboratory, JINR, Dubna, Russia, November 2006)
Short Term:
Prof. Richard Zare (Stanford University)

Current Research Activities:

Cluster Simulations and Phase Transitions, Nanoscience
Density Functional and Ab-initio Theory
Electroweak Electronic Structure Theory (Parity Nonconservation in Chiral Molecules)
Heterogeneous and Homogeneous Catalysis
Quantum Chromodynamics
Relativistic Quantum Chemistry
Simulation of Bose-Einstein Condensates
Solid State Physics
Superheavy Elements
Theoretical Inorganic and Organic Chemistry

Grants Received/Continuing

- P. Schwerdtfeger : Marsden Fund (2003-06), year 3, NZ$ 210,000 per annum
Title: *Nanostructures of Gold – From Low-Dimensional Assemblies to Heterogeneous Catalysis*
- Behnam Assadollahzadeh received NZ$ 6,000 from Education New Zealand Trust, NZ Postgraduate Study Abroad Award 2006, to visit the research group of Prof. Rolf Schäfer at the Technical University of Darmstadt (11/09-30/11/2006). He also received NZ$400 to participate at the NZIC2006 conference in Rotorua.
- Susan Biering received NZ$ 3,500 from the New Zealand Postgraduate Study Abroad Awards (NZPSAA) to visit the Center for Computational Materials Science, Vienna University of Technology, Vienna (07.08 - 18.08.2006 and 28.08 - 06.10.2006), and the Max Planck Institute for the Physics of Complex Systems, Dresden (21.08.2006 - 25.08.2006 and 16.10 - 20.10.2006), and NZ$400 to participate at the NZIC2006 conference in Rotorua.
- J. Brand received $25,000 start-up grant from IFS, Massey University.
- Andreas Hermann received NZ$ 2,500 from Education New Zealand Trust, NZ Postgraduate Study Abroad Award 2006, to visit the University of Paderborn (group of Prof. W.G. Schmidt, 01/09 - 31/10/2006), NZ$1,200 from the Graduate Research Fund, IFS, Massey University to participate at ECOSS-24, Paris, France, NZ$1,000 from IFS, Massey University to participate at the ICCMSE-2006 meeting in Greece, NZ$400 to participate at the NZIC2006 conference in Rotorua. He also received a NZ International Doctoral Research Scholarship from the Education New Zealand Trust worth NZ$ 18,000 p.a. from 01/2007 on.
- Christian Thierfelder received NZ$ 3,500 from the New Zealand Postgraduate Study Abroad Awards (NZPSAA) to visit research group of Prof. Trond Saue at the University Strasbourg (20/08 -15/09/2006), Prof. Luuk Visscher's group at the University of Amsterdam (16/09 - 15/10/2006), and Prof. Gero Schmidt's group at the University Paderborn (20/08 - 15/09/2006).
- P. Schwerdtfeger received NZ$ 2,700 form the ISAT linkage Fund to visit the University of Stuttgart.
- Both J. Brand and P. Schwerdtfeger received funding from Massey University for long-term international visitors.

Awards:

M. Lein: Coordination Chemistry Reviews: *Most cited paper* 2003-2006 for a 'top-50 most cited' paper.
Nicola Gaston (former PhD student): International Conference on Computational Science and Engineering, *Young Scientist Excellence Award for 2006* for her work on Ab initio correlation calculations for the lattice structures of Zn, Cd, and Hg carried out at Massey University.
P. Schwerdtfeger was awarded the 2007 Australasian Lectureship.

Ongoing PhD Theses

Behnam Assadollahzadeh (PhD thesis): *Properties of metal clusters of Au, Cs and Sn*.
Supervisor: P. Schwerdtfeger.
Susan Biering (PhD thesis): *Relativistic structure changes in group 12 oxides*.
Supervisor: P. Schwerdtfeger.
Andreas Hermann (PhD thesis): *Adsorption properties of water surfaces*.

Supervisor: P. Schwerdtfeger.
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 *J. Brand*
- Invited talk: "Solitons in Bose-Einstein condensates", Dodd-Walls Symposium at the University of Auckland (December 9-11, 2006).
- Invited talk: "Quantum chemistry of matter-wave solitons", NZIC (New Zealand Institute of Chemistry) Conference, Rotorua, New Zealand (December 2-6, 2006).
- Invited talk: "Quantum reflection and dissipative motion of matter-wave solitons", SOLIQUANTUM'06 (September 27-30, 2006); Also served as session chair.
- Talk: "Emergence of Superfluidity in the Dynamics of a Bose-Einstein Condensate in a Parabolic Lattice" German Physical Society(DPG) Spring Meeting, Dresden (March 30, 2006).

Given by *M. Lein*
- Invited talk: "Relativistic Pseudopotential Calculations for Catalytic Calculations of Au(III)", International Conference of Computational Methods in Sciences and Engineering (ICCMSE), Crete, Greece (October 27 – November 1 2006).

Given by *E. Pahl*
- Invited talk: "Calculation of Band Structures using Wave-Function based Correlation Methods", NZIC (New Zealand Institute of Chemistry) Conference, Rotorua, New Zealand (December 2-6, 2006).

Given by *P. Schwerdtfeger*
- Invited plenary: "Kepler's Conjecture, Newton's Kissing Problems and How to Pack Rare Gas Atoms", Theoretical Chemistry Symposium, Rauischholzhausen (Marburg), April 11-13, 2006.
- Invited talk: "The Search for Absolute Chirality", 43. ACS National Meeting, San Francisco, September 10-14, 2006.
- International Conference of Computational Methods in Sciences and Engineering (ICCMSE), Crete, Greece (October 27 – November 1 2006); Symposium organizer and session chair.

Given by *T. Söhnel*
- Invited talk: "Relativistic Effects in Solid State Structures", International Conference of Computational Methods in Sciences and Engineering (ICCMSE), Crete, Greece (October 27 – November 1 2006).

Seminars

- P. Schwerdtfeger talks at University of California, Berkeley (13/12/2006), The Lawrence Berkeley Laboratory (14/12/2006), a GDCh Lecture at the University of Würzburg, and the Mez-Starck Lecture at the University of Ulm (25/04/2006).
- J. Brand gave talks at Massey University, Albany and Palmerston North. He also gave invited talks at Harvard University, Ecole Normale Superieure (Paris), Australian National

University (Canberra), and the Universities of Otago, Auckland, Durham (UK), and Regensburg (Germany).
- P. Bowman gave seminars at Indiana University and at Massey in Albany and Palmerston North.
- M. Lein gave a research seminar at the Goethe Universität in Frankfurt.
- A. Hermann gave an invited conference talk on at the NZIC Conference 2006 in Rotorua.
- E. Pahl gave a talk at Massey University (Albany).
- C. Thierfelder gave presentations at the 9th Dirac Meeting, University Odense (14/08/2006), at the University Strasbourg (12/09/2006), and at the University of Amsterdam (10/10/2006).

Posters

Poster session at the International Conference of Computational Methods in Sciences and Engineering (ICCMSE), Crete, Greece (October 27 – November 1 2006):
- B. Assadollahzadeh, S. Schäfer, P. Schwerdtfeger, "Polarizabilities of medium-sized tin clusters (Sn_{10}-Sn_{18}): A DFT Study".
- S. Biering, A. Hermann, W. G. Schmidt, "A Density functional approach to the adsorption of water on chlorine-terminate Si(111)".
- A. Hermann, P. Schwerdtfeger, "Magnetic Properties of α-$CrCl_2$: Benchmarking first principles methods".
- C. Thierfelder, P. Schwerdtfeger, "Relativistic effects in superheavy hydrides".

Poster session at the NZIC (New Zealand Institute of Chemistry) Conference, Rotorua, NZ (December 2-6, 2006):
- B. Assadollahzadeh, S. Schäfer, P. Schwerdtfeger, "Polarizabilities of medium-sized tin clusters (Sn_{10}-Sn_{18}): A DFT Study".
- S. Biering, A. Hermann, W. G. Schmidt, "A Density functional approach to the adsorption of water on chlorine-terminate Si(111)".
- A. Hermann, P. Schwerdtfeger, "Magnetic Properties of α-$CrCl_2$: Benchmarking first principles methods".
- P. Schwerdtfeger, G. Moyano, "The Rare Gas Packing Problem".
- B. Vest, P. Schwerdtfeger, "The Electronic and Structural Properties of Gas-phase Chromium(II) Dihalide Clusters".

Other work

Papers refereed:
- P. Bowman refereed papers for Physical Review D and Physical Review Letters.
- M. Lein is regular referee of the Journal of Computational Chemistry.
- P. Schwerdtfeger refereed 55 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.)

Community Outreach: P. Bowman and J. Brand served as judges for the Murray's Bay Intermediate School Science Fair.
PhD and MSc theses refereed: P. Schwerdtfeger reviewed the BSc honours thesis of Ross James Davidson, IFS, Massey University (23/11/2006).

PUBLISHED WORK

Papers published in refereed journals

1. R. Bast, P. Schwerdtfeger, T. Saue, " Parity non-conserving contribution to the NMR shielding constants of chiral molecules: A 4-component relativistic study", ***J. Chem. Phys.*** 125, 064504-1-7 (**2006**).

2. S. Biering, A. Hermann, W. G. Schmidt, "Adsorption of water on chlorine-terminated Si(111) from first principles: Substrate-induced ordering versus intermolecular interactions", ***Phys. Rev. B*** 73, 235429-1-6 (**2006**).

3. J. Brand and A. R. Kolovsky, "Emergence of superfluid transport in a dynamical system of ultra-cold atoms", ***Europhys. J. D*** 38, 85-91 (**2006**).

4. Yu. Cherny and J. Brand, "The polarizability and dynamic structure factor of the 1D Bose gas near the Tonks-Girardeau limit at finite temperatures", ***Phys. Rev. A*** 73, 023612-1-12 (**2006**).

5. N. Gaston, P. Schwerdtfeger, T. Saue, J. Greif, "The frequency-dependent dipole polarisability of the mercury dimer from four-component relativistic density functional theory", ***J. Chem. Phys.*** 124, 044304-1-7 (**2006**).

6. N. Gaston, P. Schwerdtfeger, "From the van der Waals dimer to the solid-state of mercury with relativistic ab initio and density functional theory", ***Phys. Rev. B***, 74, 024105-1-12 (**2006**).

7. N. Gaston, B. Paulus, K. Rosciszewski, P. Schwerdtfeger, H. Stoll, "The lattice structure of mercury: Influence of electronic correlation.", ***Phys. Rev. B*** 74, 094102-1-9 (**2006**).

8. N. Gaston, P. Schwerdtfeger, B. v. Issendorff, "The photoabsorption spectra of cationic mercury clusters". ***Phys. Rev. A*** 74, 094102-1-9 (**2006**).

9. A. Hermann, B. Vest, P. Schwerdtfeger, "Density functional study of α-$CrCl_2$: structure, electronic and magnetic properties", ***Phys. Rev. B*** 74, 224402-1-7 (**2006**).

10. R. P. Krawczyk, A. Hammerl, and P. Schwerdtfeger, "Nucleation of Coinage Metal Halides - When Clusters Start to Converge Towards the Solid State Structure", ***Chem. Phys. Chem.*** 7, 2286-2289 (**2006**).

11. Ch. Lee, J. Brand, "Enhanced Quantum Reflection of Matter-Wave Bright Solitons", ***Europhys. Lett.*** 73, 321-327 (**2006**).

12. I. S. Lim, H. Stoll, P. Schwerdtfeger, "Relativistic Small-Core Energy-Consistent Pseudopotentials for the Alkaline-Earth Elements from Ca to Ra", ***J. Chem. Phys.*** 124, 034107-1-9 (**2006**).

13. E. Pahl, U. Birkenheuer, "Frozen local hole approximation", ***J. Chem. Phys.*** 124, 214101 (**2006**).

14. M. Parappilly, P. Bowman, U. Heller, D. Leinweber, A. Williams, J. Zhang, "Scaling behavior of quark propagator in full QCD", ***Phys. Rev. D*** 73, 054504 (**2006**).

15. G. Rauhut, V. Barone, P. Schwerdtfeger,"Vibrational Analyses for CHFClBr and CDFClBr Based on High Level Ab Initio Calculations", ***J. Chem. Phys.*** 125, 054308-1-7 (**2006**).

16. P. Schwerdtfeger, N. Gaston, R. P. Krawczyk, R. Tonner, G. E. Moyano, "Theoretical investigations into rare gas clusters and crystal lattices of He, Ne, Ar and Kr using many-body interaction expansions – the Lennard-Jones Potential revised", ***Phys. Rev. B*** 73, 064112-1-19 (**2006**).

17. S. Sinha, A. Yu. Cherny, D. Kovrizhin, J. Brand, "Friction and Diffusion of Matter-Wave Solitons", ***Phys. Rev. Lett*** 96, 030406-1-4 (**2006**).

18. C. Thierfelder, A. Hermann, P. Schwerdtfeger, W. G. Schmidt "Strongly bound water monomers on the Ih basal plane: First-principles density functional calculations", ***Phys. Rev. B*** 74, 045422-1-5 (**2006**).

Conference Proceedings

1. P. Bowman, U. Heller, D. Leinweber, M. Parappilly, A. Williams, "QCD propagators: some results from the lattice" in "LC 2005", Nuclear Physics B (Proc. Suppl.) 161 (**2006**); pg. 27-33.

2. D. Leinweber, P. Bowman, U. Heller, D-J. Kusterer, K. Langfeld and A. Williams, "Role of centre vortices in dynamical mass generation" in LC 2005, Nuclear Physics B (Proc. Suppl.) 161 (**2006**); pg. 130-135.

3. M. Parappilly, P. Bowman, U. Heller, D. Leinweber, A. Williams, J. Zhang, "*Effects of dynamical sea-quarks on quark and gluon propagators*" in "*PARTICLES AND NUCLEI: Seventeenth International Conference on Particles and Nuclei*", AIP Conference Proceedings Volume 842 (**2006**); pg. 237-239.

4. P. Schwerdtfeger, C. Thierfelder, "*Relativistic Quantum Chemistry – A Historical Overview*." In *Trends and Perspectives in Modern Computational Science***,** in *Lecture Series on Computer and Computational Sciences*, eds. G. Maroulis, T. Simos, Volume 6, Brill Academic Publishers, Leiden, The Netherlands (**2006**); pg.453-460.

Book chapters:

P. Schwerdtfeger, "Atomic Static Dipole Polarizabilities", in *Computational Aspects of Electric Polarizability Calculations: Atoms, Molecules and Clusters,* ed. G. Maroulis, IOS Press, Amsterdam (**2006**); pg.1-32.

Books edited:

M. Lein (editor) "Proceedings of the NZIC 2006", The New Zealand Institute of Chemistry (2006), ISBN 978-0-473-11854-9. 450 pages

Prof. Peter Schwerdtfeger
Date: March 9, 2007