



Centre for
T H E O R E T I C A L
Chemistry and Physics



Massey University

CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
NEW ZEALAND INSTITUTE FOR ADVANCED STUDY
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To: Prof. Robert Anderson (PVC)

CTCP ANNUAL PERFORMANCE REPORT 2008

Activities and achievements: 2008 was again a most successful year for our CTCP. We saw the arrival of three new postdoctoral fellows (Beata Dabrowska-Wüster, Renyuan Liao and Ralf Tonner), two of our members moved from PhD to postdoctoral positions (Behnam Assadollahzadeh took up a Marsden fellowship, and Brian Vest is on a 0.5 postdoctoral fellowship). Ralf Tonner finished his DAAD fellowship and was able to secure two more years on an Alexander von Humboldt Feodor-Lynen fellowship starting in 2009. The CTCP chemistry group moved out of the Institute of Fundamental Sciences (IFS) into the New Zealand Institute for Advanced Study (IAS). We hosted a number of eminent international visitors and will continue to do so. The long-term visitors received funding from the international visitors fund of Massey University.

In July 2008 we saw 5 Marsden grants running and one new coming (in collaboration with Victor Flambaum, also a member of the IAS) on “The Variation of Fundamental Constants in Space-Time”, starting January 1 2009 (PI: P. Schwerdtfeger, V.V.Flambaum; NZ\$ 780,000 over three years). This grant was one of the largest in the country. In fact, in 2009 our centre will run 6 Marsden grants in total, unmatched by any other research centre in New Zealand. This clearly demonstrates the excellence of science carried out here in Albany. Andreas Hermann handed in his PhD thesis (proof stage) on “Ab-initio calculations of water and ice: structural, electronic, and optical properties”. Two of our PhD students (Susan Biering and Christian Thierfelder) are currently writing up their PhD theses.

Massey University took delivery of its 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 computer ran without major down-time again for the whole year in 2008, which reflects the quality of hardware provided by the Insite group in Christchurch. The current system is running at maximum capacity, and to complete more research, compute jobs must be queued until other jobs are completed, delaying important research output. Moreover, this machine is now 4 years old and at the absolute end of its intended lifetime. Even with the BestGrid machine on-line, which is running at 0% idle time, it cannot satisfy our computational needs. High performance computing at Massey University represents a significant research infrastructure resource to our centre (and to the wider computing community at Massey University) that needs to be maintained and significantly enhanced. In fact, the computational facility in Albany leads to more papers published in top journals than any other facility at Massey University. Chris Messom at IIMS prepared a business case for a

large compute cluster called Helix³, and we are eagerly awaiting the first implementation stage of this important computational facility. Furthermore, a software analyst is required to maintain the software for our machines.

All members of CTCP were involved in chemistry and physics teaching. Behnam Assadollahzadeh was involved in tutorials and student supervision. P. Bowman taught stage 2 digital electronics. J. Brand taught stage 1 physics during semesters one and two in Albany. D. Figgen was involved in lab-supervision at the stage 1 level in chemistry and in the supervision of exchange students. M. Lein was involved in lab-teaching and lectured at stage 1 level in Chemistry. E. Pahl was involved in first year 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 of *Introduction to Quantum Theory* for the year 3 Physical Chemistry course, and five lectures on *Chemical Evolution* in the stage 2 paper on Evolution Theory in Biological Sciences. U. Zülicke taught physics papers in Palmerston North at all levels.

Other activities: P. Bowman served on the IFS Strategy Committee. J. Brand served on the IFS Research and Equipment Committee and on the IFS Management Committee. U. Zülicke served on the IFS Programmes Committee and took on responsibility as the Physics Subject Leader. M. Lein served on the Science Building Planning Committee and the Workplace Health and Safety Committee. P. Schwerdtfeger served as the President of the New Zealand Alexander von Humboldt Association, was on the board of the Asian Pacific Theoretical & Computational Chemistry Society and the Albany Academic Committee, and finished his last year of membership on the Council of the Royal Society of New Zealand. He is also on the editorial board of *Journal of Computational Chemistry*, *Structural Chemistry*, *Journal of Structural Chemistry (Theochem)*, and *Lecture Series on Computer and Computational Sciences*. Thomas Ernst served on the IFS Postgraduate Committee.

Research Highlights: In collaboration with Florent Calvo (Lyon) we are simulating the melting behaviour of large rare gas clusters. We succeeded to be within 1.0 Kelvin of the experimental melting temperature of Argon for the first time, which has not been achieved so far. This work is now published in *Angewandte Chemie*, a journal with an impact factor over 10. For the first time we were also able to explain the onset of optical absorption of water, which is blue-shifted upon condensation and substantially opens the far-UV window. Furthermore, we were able to model solid water for the first time using ab-initio techniques. Both research outcomes are now published in *Physical Review Letters*, the physics journal with the highest impact factor. The latter work was discussed in the online edition of the journal *PhysicsWorld*, and will be discussed in the journal of the German Physical Society, *PhysikJournal*. On the parity violation front we investigated a promising class of small but heavy chiral compounds. In collaboration with Sergej Flach (Dresden) and Larry Schulman (New York) we investigated the influence of quantum entanglement between bosonic atoms in the formation of nonlinear localised modes of ultra-cold atoms in an optical lattice. We found that entanglement can be crucial to the extent that localization would not be possible without it. These results are now published in *Europhysics Letters*. We have made further progress in understanding novel spin physics in *p*-type semiconductor nanostructures, finding intriguing properties of hole spin splitting and the existence of an anomalous Berry phase that could be measured in mesoscopic hole rings. These findings are published in several articles that appeared in *Applied Physics Letters* and *Physical Review B*. In collaboration with researchers at Adelaide and Southampton, centre vortices were seen to have little effect on chiral symmetry breaking in QCD, while entirely accounting for it in SU(2) gauge theory. This presents a significant challenge for the popular centre vortex model. This work was published in *Physical Review D*, with a follow-up publication to be submitted shortly. One of our students, C. Thierfelder was an invited visiting fellow (12/10/2008 - 18/11/2008) at the University of New South Wales, Sydney.

Future opportunities and directions: The double-helix supercomputer at Albany is hopefully (!) being upgraded in 2009. We aim for The Helix³ – A Shared/Distributed (4x32, 8x16, 16x8) Parallel Compute Cluster, 4 Distributed Units of 32 Shared Cores with a total of 128 Cores (32 quad-core processors), 8 Distributed Units of 16 Shared Cores with a total of 128 Cores (32 quad-core processors), 32 Distributed Units of 8 Shared Cores with a total of 256 Cores (64 quad-core processors). These will form a Compute Parallel Cluster connected by Infiniband. Each 32 core node contains 128 Gbyte RAM (4 GB per core) for high RAM required computations. The 16 core nodes will contain 64GB RAM (4 GB per core), while the 8 core nodes will contain 32GB of RAM (4GB RAM per core). Each node will contain 1 small partition for the operating system and 4x1 Tbyte disk space for the cluster file system and the scratch files. 1 large uninterrupted power supply (UPS) and 1 switch are needed to run the cluster. Annual running costs include salary for 1 system administrator.

Two buildings (40 and 44) at Oteha Rohe still urgently require air-conditioning as the working environment in summer becomes unbearable in the huts occupied due to the additional heat generated by the many high powered computer workstations. This year we experienced again 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 with each unit producing 0.5 kWh in heat. We are now installing an air-conditioning system for the server room in building 44, so at least the server is not overheating. The money for this air-conditioning system comes from the IAS.

We also need more space for the additional postdoctoral workers and PhD students joining our centre. The picture below shows a snap-shot of our research group. With 20 or more people distributed over 2 huts, there is no space left for increasing our research activities. We are basically stretched to the limit. Despite of what we hear (“There are no space problems of Oteha Rohe”), it is utterly frustrating for us sitting in overcrowded “hot”-houses.

Another frustrating point is that our centre is split right through the middle as half of us belong to IAS, the other to IFS, with two secretaries with “complementary” duties. We are all looking forward being part of the new Institute for Natural Sciences (INS) at Albany.

Performance against objectives: All objectives were met as we are one of the most productive research centres here in New Zealand, with truly outstanding performances by each of our staff members. All papers published are in highly acclaimed international journals of high impact factor. One major Marsden grant was received in 2008, and we hope for more in 2009.

In summary, it was a great year for our centre. I believe that, in comparing ourselves with other research centres in New Zealand, which are often much larger in size than ours with far more research funding, we have achieved a very high international standing only matched by top research institutes world-wide. This is reflected by the many invitations to present talks overseas, and by the many high-standing visitors who come to our research centre. Finally, my very special thanks goes to our Institute’s secretary, Mrs. Vesna Davidovic-Alexander (now IAS), who has helped us so much to run the centre, organizing conferences, looking after our visitors and many more.



Prof. Peter Schwerdtfeger

Date: December 9, 2008

Cc: Hon. Steve Maharey (VC)
Prof. Nigel Long (DVC)
Prof. G. Martin (IAS)
Prof. P. Derrick (IFS)

Appendix



From the left to the right:

Elke Pahl, Phil Bunker, Claudia Loerbrok, Anton Koers, Dee Debbage, Beata Dabrowska-Wüster, Thomas Ernst, Peter Schwerdtfeger, Matthias Lein, Ralf Tonner, Joachim Brand, Andreas Hermann, Patrick Bowman, Philip Bron, Renyuan Liao, Detlev Figgen, Brian Vest, Susan Biering, Behnam Assadollahzadeh, Vesna Davidovic-Alexander

Missing in this picture: Christian Thierfelder, Tilo Söhnel, Uli Zülicke (Palmerston North)

Personnel

Prof. Peter Schwerdtfeger (Director of CTCP)
Assoc. Prof. Joachim Brand (Deputy Director of CTCP)
Assoc. Prof. Uli Zülicke (based in Palmerston North)
Dr. Patrick Bowman (Senior Lecturer)
Dr. Matthias Lein (Research Officer)

Secretaries

Vesna Davidovic-Alexander (IAS)
Dee Debbage (IFS)

Postdoctoral Fellows

Dr. Behnam Assadollahzadeh (Marsden fellow)
Dr. Beata Dabrowska-Wüster (Marsden fellow)
Dr. Detlev Figgen (Marsden fellow)
Dr. Renyuan Liao
Dr. Elke Pahl
Dr. Ralf Tonner (DAAD fellow)
Dr. Brian Vest (since July 1)

PhD Students

Susan Biering
Thomas Ernst
Andreas Hermann
Christian Thierfelder
Brian Vest

Exchange Students

Anton Koers (Vrije Universiteit Amsterdam)
Philip Bron (Philipps Universität Marburg)
Claudia Loerbrok (Philipps Universität Marburg)
Love Koci (Uppsala University, Sweden)
Kathrin Schaffert (Ruhr-Universität Bochum)

Honorary Research Fellows

Dr. Tilo Söhnle (Senior Lecturer, Auckland University)

Visitors from other institutions:

Long Term:

Prof. Phil Bunker (NRC, Ottawa Canada, November 1-30)
Dr. Florent Calvo (Université Claude Bernard Lyon, France, March 1-31)
Prof. Robert Glaser (Ben-Gurion University, Israel)

Short Term:

Prof. Jim Colman (Stanford University, USA)
Prof. Robert Graham (University of Duisburg-Essen, Germany)
Prof. Ekkehard Hahn (Münster University, Germany)
Dr. David Hallwood (University of Leeds, UK)
Dr. David Hutchinson (University of Otago)

Current Research Activities:

Cluster Simulations and Phase Transitions, Nanoscience
Density Functional and Ab-initio Theory
Transition Metal Catalysis and Theory of Chemical Bonding
Electroweak Electronic Structure Theory (Parity Nonconservation in Chiral Molecules)
Heterogeneous and Homogeneous Catalysis
High-Pressure Physics
Quantum Chromodynamics
Relativistic Quantum Chemistry
Simulation of Bose-Einstein Condensates
Quantum dynamics of ultra-cold few-atom systems
Solid State Physics
Superheavy Elements
Theoretical Inorganic and Organic Chemistry
Theory of functional nanostructures; Spintronics

Grants Received/Continuing

- P. Bowman in his second year on his Marsden grant “How hadrons keep their quarks“ NZ\$85,000 per annum.
- J. Brand is receiving Marsden funding (together with H-D. Meyer and P. Schmelcher from University of Heidelberg as AIs) for the project “Few-body dynamics of ultra-cold atoms” (2008-2010) NZ\$670,000 in total, which started in February 2008 (MAU0706).
- P. Schwerdtfeger received a Marsden grant (together with V.V. Flambaum, Member of IAS) for the project “The Variation of Fundamental Constants in Space-Time” (2009-11), NZ\$ 260,000 per annum for 3 years (08MAU070). He continues on two other Marsden grants as principal investigator, “Chemistry at extreme conditions: materials at ultra-high pressures from first principles quantum theoretical methods”, NZ\$ 240,000 per annum (07MAU016), and “The search for molecular parity violation – precise four-component relativistic coupled cluster and density functional calculations of parity non-conservation effects in chiral molecules”, NZ\$ 290,000 per annum (07MAU016).
- U. Zülicke received funding from the 2008 NERF round as a subcontractor on two projects commencing in 2009: “Rare-earth nitride spintronics devices” (VUW/IRL collaboration) and “Magnetic nanoclusters” (GNS collaboration). He also continues his Marsden grant (contract MAU0702).

Awards

- A. Hermann was awarded the “Poster Prize” (A\$ 100) at the WATOC 2008 conference in Sydney, September 2008.
- T. Ernst was awarded the Student's choice for best talk at the IFS Postgraduate Research Symposium, Massey University Palmerston North (February 20).
- R. Tonner received a Feodor-Lynen fellowship of the German Alexander von Humboldt Foundation as post-doctoral funding for 2 years.
- U. Zülicke was awarded the NZ Association of Scientists Research Medal for 2008.

Ongoing PhD Theses

- S. Biering: *Relativistic structure changes in group 12 oxides*. Supervisor: P. Schwerdtfeger.
- T. Ernst: *Time dependent many-body theory for degenerate quantum gases*. Supervisor: J. Brand. Thomas Ernst also passed the examination for the 1st year confirmation as doctoral candidate.
- A. Hermann: *Ab-initio calculations of water and ice: structural, electronic, and optical properties*. Supervisor: P. Schwerdtfeger.
- C. Thierfelder: *Applications to the Dirac equation – from relativistic effects to electroweak interactions*. Supervisor: P. Schwerdtfeger.

Finished PhD Theses

- B. Assadollahzadeh: *Properties of metal clusters of Au, Cs and Sn*. Supervisor: P. Schwerdtfeger.
- B. Vest: *Nucleation of chromium dihalides – from the gas phase to the solid state*. Supervisor: P. Schwerdtfeger.

Lectures at Conferences / Meetings

P. Bowman

- Invited talk at Confinement and the Hadron Spectrum 8, Mainz, Germany, September 1-6, 2008. Title: "Centre vortices and the quark propagator".
- Invited talk at Approaches to Quantum Chromodynamics, the 419th W.E. Heraeus Seminar, in Oberwoelz, Austria, September 7 - 13, 2008. Title: "Lattice QCD Green's Functions as Probes of Dynamical Chiral Symmetry Breaking and Confinement".

J. Brand

- Invited talk at the ACQAO meeting *Quantum optics beyond Bells*, Lorne (Victoria), Australia (Nov. 2008). Title: "Topological Solitons in Double-Ring Bose-Einstein Condensates".
- Invited talk at the conference *Nonlinear phenomena in degenerate quantum gases*, Toledo, Spain (April 2008). Title: "Phase Diagram of Double-Ring BECs".
- Invited talk at the *Dodd-Walls Centre Symposium*, Dunedin (February 2008). Title: "Correlated Quantum Dynamics of Few Particles".
- Talk at the conference *Nonlinear Waves 2008 – Theory and Applications*, Beijing, China (June 2008). Title: "Phase Diagram of Double-Ring BECs".
- Talk at the *Dodd-Walls Symposium*, Queenstown (December 2008). Title: "Topological Solitons in Double-Ring Bose-Einstein Condensates".

M. Lein

- Invited talk at the WATOC 2008 meeting in Sydney, Tue. 16 Sep. "Theory and Experiment of Linear Agostic Interactions: A New Motif in and Old Concept".
- Invited talk at the NZIC Meeting 2008 in Dunedin, Fri. 5 Dec. "The Determining Effects of Relativity on the Homogeneously Au(III) Catalysed Addition of Water to Propyne".
- Invited talk at the IC08 Meeting 2008 in Christchurch, Tue. 16 Dec. "The Effects of Relativity on Reaction Mechanisms – Gold(III) Catalysis as an Example".

P. Schwerdtfeger

- Two keynote lectures at the conference on *50 years of coupled cluster theory*, INT, Seattle, USA, June 30 – July 2, 2008. Title of the talks: i) "Nuclear Multipole Moments from Electronic Structure Theory", and ii) "The Search for Parity Violation in Chiral Molecules".
- Two Plenary Talks at the International WE Heraeus Summer School: Atomic Properties of the Heaviest Elements, Wittenberg, Germany, August 24–September 6, 2008. Title of the talks: i) "Relativistic and QED Effects in Heavy and Superheavy Elements. Part 1. Relativistic Quantum Theory", and ii) "Relativistic and QED Effects in Heavy and Superheavy Elements. Part 1. Bound State QED".
- Keynote lecture at the Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC08), Sydney, Australia, September 14–19, 2008. Title of the talk: "Chromium Dihalides – A Challenge to Computational Chemistry".
- Keynote Lecture at the 5th IIMS Post Graduate Conference, Auckland, October 23, 2008. Title of the talk: "Kepler's Conjecture, Newton's Kissing Problems and How to Pack Atoms".
- Keynote lecture at the Kernz08, International Conference on Interfacing Structure and Reactions at the Centre of the Atom, Queenstown, New Zealand, December 1–5, 2008. Title of the talk: "Nuclear Multipole Moments from Relativistic Electronic Structure Theory".
- Keynote lecture Gas Phase Ion Chemistry: State of the Art and Perspectives, An International Symposium in Honour of Prof. Dr. Helmut Schwarz, President of the Alexander von Humboldt Foundation, Kloster Eberbach, Germany, December 14–16, 2008. Title of the talk: "From the Solid to the Liquid Phase - Towards the Prediction of Accurate Melting Temperatures for the Rare Gas Elements".

R. Tonner

- Invited talk: "Are carbodiphosphoranes better ligands than N-heterocyclic carbenes for Grubbs' catalysts?", Hood Fellow Symposium, University of Auckland, Auckland/New Zealand, April 2008.
- Invited talk: "Adsorption of proline and glycine on the TiO₂(110) surface – a DFT study", IC08, Christchurch/New Zealand, December 2008.

U. Zülicke

- Invited talk at the International Workshop on Spin Phenomena in Reduced Dimensions, Regensburg, Germany, 24–26 September 2008. Title of the talk: "Spin-related geometric phase in mesoscopic hole rings".
- Invited talk at the International Symposium Nanoelectronics and Quantum Transport, Karlsruhe, Germany, 18–19 April 2008. Title of the talk: "Spin splitting, polarisation, and geometric phase of quantum-confined holes".
- Invited talk at the Villa & Virtual Joint Conferences on Interaction Among Nanostructures, Orlando, Florida, USA, 3–7 February 2008 (talk was delivered from New Zealand via the WWW). Title of the talk: "Spin splitting and polarisation in hole nanowires".
- Talk at the 2008 International Conference On Nanoscience and Nanotechnology (ICONN 2008), Melbourne, Australia, 25 – 29 February 2008. Title: "Nanospintronics meets relativistic quantum physics: Ubiquity of Zitterbewegung effects".

Seminars and Talks

- S. Biering: Seminar on “The unusual structure of mercury oxide: A first principles density functional study for the group 12 oxides”, CTCP seminar series, Massey University, November 2008.
- P. Bowman gave a series of advanced lectures on Quantum Field Theory at Massey University.
- J. Brand gave invited seminar talks at the Institute of Physics of the Chinese Academy of Sciences, Beijing (13/6/2008). Title: “Fano Resonances in Atom Scattering on a BEC”; at the University of Science and Technology Beijing (6/6/2008). Title: “Solitons and Vortices in Bose-Einstein Condensates”; and at the University of Heidelberg, Germany (28/4/2008). Title: “Fluxons in Double-Ring Bose-Einstein Condensates”.
- T. Ernst gave a talk at the annual IFS Postgraduate Research Symposium “Trapping of matter-wave solitons”, Massey University Palmerston North (February 20). He also gave an invited talk “Resonant trapping in the transport of a soliton through a quantum well” at the complex quantum systems group seminar, physics department, University of Regensburg (June 11), and a talk at the CTCP seminar “Dynamics of solitons in quantum gases” (August 8).
- D. Figgen: Seminar on the adjustment and application of relativistic pseudopotentials, CTCP seminar series, Massey University Albany, Auckland/New Zealand, March 2008
- A. Hermann: Seminar on “Ab-initio calculations of water and ice”, CTCP seminar series, Massey University, October 2008.
- M. Lein, Seminar in the CTCP lecture series: “Recent work: Agostic Interactions, a new Motif in an Old Concept and Relativistic Effects in Gold (III) Catalysis, Addition of Water to Propyne.”
- E. Pahl: Invited seminar talks in Stuttgart (8/4) and Berlin (22/4) on “Melting of nano clusters”
- P. Schwerdtfeger gave a professorial public lecture on “ ‘Everything is relative’, says Albert Einstein, and we chemists are learning it the hard way!” in the Sir Neil Waters Lecture Theatre Building, March 6. Seminars in Albany: “Biomolecular Homochirality – A Necessary Condition for Life” (April 9). Invited talks at the Universities in Heidelberg (“The Search for Parity Violation Effects in Chiral Molecules”, April 21), Ulm (“Pseudopotential Theory”, April 25), FU Berlin (GdCH Talk on “The Search for Parity Violation Effects in Chiral Molecules”, May 5), Washington Seattle (“Relativistic Effects in the Solid State”, June 27).
- C. Thierfelder gave invited seminar talks at the School of Physics at the University of New South Wales, Sydney (30/10/2008). Title: “Radiative potentials and atomic many-body theory”
- R. Tonner: Seminar on Divalent carbon(0) chemistry of carbodiphosphanes and analogues, CTCP seminar series, Massey University Albany, Auckland/New Zealand, April 2008
- U. Zülicke gave an invited seminar/colloquium lecture entitled “Nanospintronics meets relativistic quantum physics: Ubiquity of Zitterbewegung effects” at the University of Otago (5 May) and at the University of Science and Technology of China (9 April), as well as a seminar lecture “Spintronics with bubbles: Spin splitting, polarisation, and geometric phase of quantum-confined holes” at the University of Science and Technology of China (3 April).

Posters

- B. Assadollahzadeh presented posters on “From Clusters to the Solid State – Global Minimum Structures for Cesium Clusters and their Electronic Properties” at the WATOC 2008, Sydney/Australia, September 2008 and “From Clusters to the Solid State – A Systematic Search for Global Minimum Structures at the RunningHot08 Conference in Wellington, November 2008.
- S. Biering presented a poster on “A first principles study of relativistic effects in bulk group 12 oxides” at the WATOC 2008, September 2008, Sydney, Australia.
- Th. Ernst presented a poster at the Dodd-Walls symposium, Dunedin, University of Otago on “Trapping of matter-wave solitons in a quantum well” (February 11-12), at the Dodd-Walls symposium, Queenstown, “Scattering of a soliton on a well” (December 9-11), and at the Cold Atom Theory workshop, Queenstown, “Scattering of a soliton on a well” (December 12).
- D. Figgen presented a poster titled “Simple but Effective: Relativistic Effective Core Potentials in Connection with Series of Correlation Consistent Basis Sets” at the WATOC 2008, Sydney, Australia.
- A. Hermann presented a poster on “Water’s Optical Spectrum: Many-body effects, Electrostatics, and Coordination”, WATOC 2008, September 2008, Sydney, Australia.
- M. Lein presented two posters “Relativistic Effects in Homogeneous Catalysis with Au(III) – Addition of Water to Propyne” and “Linear Agostic Interactions – Is side-on coordination necessary?” at the WATOC 2008 in Sydney, Sep 2008.
- E. Pahl presented a poster on “Melting of nanoclusters” at the WATOC 2008, September 2008, Sydney, Australia
- C. Thierfelder presented a poster titled “Identification of superheavy elements by gamma-spectroscopy” at the WATOC 2008, Sydney, Australia
- R. Tonner presented posters on “Are carbodiphosphoranes better ligands than N-heterocyclic carbenes for Grubbs' catalysts?” at the WATOC 2008, Sydney/Australia, September 2008, and on “Adsorption of glycine and proline on the TiO (110) surface”, at the WATOC 2008 Satellite meeting, Auckland/New Zealand, September 2008.

Teaching

- P. Bowman taught 124.242/252, stage 2 course on Digital Electronics and part of 124.101, stage 1 physics.
- J. Brand taught parts of 124.101 and 124.102, stage 1 physics.
- M. Lein taught 124.101 (Lab course) and 124.102 (Lectures) stage 1 Chemistry
- P. Schwerdtfeger taught Thermodynamics stage 1 physics (124.102) and Chemical Evolution in the Evolution paper (196.207), also 2 papers in Palmerston North, Chemical Physics stage 3 and Theoretical Chemistry stage 4.
- U. Zülicke taught half of the undergraduate physics papers 124.102, 124.226, and 124.327, the entire postgraduate paper 124.712, and 6 lectures in 236.201 Nanoscience.

Other activities

Papers refereed:

- P. Bowman refereed papers for Phys. Rev. Lett., and Few Body Systems.
- J. Brand refereed papers for the journals Phys. Rev. Lett., Phys. Rev. A, J. Phys. A, J. Phys. B, New Journal of Physics, Physica Scripta, Physica D, and Fluid Dynamics Research. Also reviewed grant applications from the Binational Science Foundation (USA-Israel) and EPSRC (UK).
- M. Lein refereed papers for Coord. Chem. Rev., J. Comput. Chem., J. Mol. Struct. THEOCHEM, IUPAC Conference Proceedings, Theor. Chem. Acc.
- P. Schwerdtfeger refereed in total 50 papers from international journals including Angewandte Chem. Int. Ed., Chem. Soc. Rev., Chem. Phys. Chem., Chem. Phys. Lett., Europ. J. Inorg. Chem., Inorg. Chem., J. Comput. Chem., J. Chem. Phys., J. Phys. Chem. A, Mol. Phys., PCCP, Phys. Rev. Lett., Phys. Rev. A, Theoret. Chem. Acc., J. Mol. Struct. (Theochem.) and many more. Also reviewed grant applications from AURC (Australia) and NSF (Switzerland).
- R. Tonner refereed papers from Journal of Computational Chemistry, Journal of Catalysis A and Journal of Fluorine Chemistry.
- U. Zülicke is a regular referee for Phys. Rev. Lett., Phys. Rev. B, Appl. Phys. Lett., Eur. Phys. J. B, Physica E.

PhD and MSc theses refereed:

- J. Brand examined a MSc thesis.
- P. Schwerdtfeger refereed a PhD thesis from Henrik Kjaergaard's group in Otago.
- P. Bowman examined a Massey University MSc thesis.
- U. Zülicke examined a Massey University PhD thesis.

Conference Organisation

- P. Bowman served on the Local Organising Committee for *QCD Downunder 2*, Massey University, Albany, January 17 - 19, 2008.
- J. Brand served as lead organiser of the Minisymposium *Nonlinear Waves in Quantum Gases* at the conference *Nonlinear Waves – Theory and Applications*, Beijing (June 2008).
- J. Brand served as co-organiser of the workshop on *Cold Atom Theory*, satellite meeting of the *Dodd-Walls Symposium*, Queenstown (12/12/2008).
- P. Schwerdtfeger, M. Lein, R. Tonner and V. Davidovic-Alexander organized the satellite meeting to the Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC08) from Sep 10 – 13 in the Spencer on Byron Hotel, Takapuna, Auckland/New Zealand with more than 25 lectures and over 50 participants.
- U. Zülicke is a member of the International Advisory Board of the 5th International School and Conference on Spintronics and Quantum Information Technology (Spintech 5).

Chairs at Conferences

- J. Brand chaired sessions at the conference *Nonlinear phenomena in degenerate quantum gases*, Toledo, Spain (April 2008), the conference *Nonlinear Waves – Theory and Applications*, Beijing (June 2008), and at the workshop on *Cold Atom Theory*, Queenstown (12/12/2008).
- P. Schwerdtfeger chaired a session at the WE Heraeus Summer School: Atomic Properties of the Heaviest Elements, in Sydney (September 14-19), and another session at the Superheavy Element Symposium in Wittenberg, Germany (August 24-September 6, 2008).

PUBLISHED WORK

Papers published in refereed journals:

1. B. Assadollahzadeh, P. R. Bunker, P. Schwerdtfeger, "The low lying isomers of the copper nonamer cluster, Cu_9 ", *Chem. Phys. Lett.* **451**, 262-269 (2008).
2. B. Assadollahzadeh, P. Schwerdtfeger, "A Comparison of Metallophilic Interactions in Group 11 $[\text{X-M-PH}_3]_n$ ($n=2-3$) Complex Halides ($\text{M}=\text{Cu}, \text{Ag}, \text{Au}$; $\text{X}=\text{Cl}, \text{Br}, \text{I}$) from Density Functional Theory." *Chem. Phys. Lett.* **462**, 222-228 (2008).
3. P. O. Bowman, K. Langfeld, D. B. Leinweber, A. O'Cais, A. Sternbeck, L. von Smekal, A. G. Williams, "Center vortices and the quark propagator in $\text{SU}(2)$ gauge theory", *Phys. Rev. D* **78**, 054509-1-7 (2008).
4. J. Brand, S. Flach, V. Fleurov, L. S. Schulmann und D. Tolkunov. "Localization by entanglement". *Europhys. Lett.* **83**, 40002 (2008).
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