



Massey University

CENTRE OF THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
INSTITUTE OF FUNDAMENTAL SCIENCES
Bldg. 40 and 44, Private Bag 102 904, North Shore MSC,
Auckland, New Zealand

To: Prof. Robert Anderson (PVC)

CTCP ANNUAL PERFORMANCE REPORT 2007

Activities and achievements: 2007 was perhaps the most successful year for our CTCP. Uli Zülicke joined the CTCP beginning of 2007. This is an important addition to our small research centre. Two members received promotion to the level of Associate Professor, Uli Zülicke and Joachim Brand. We saw the arrival of one new PhD student (Thomas Ernst) and one postdoctoral fellow (Detlev Figgen). We also hosted a number of eminent international visitors. And our web-site is up and going, check: <http://ctcp.massey.ac.nz>.

In July 2007 the Marsden grant on nano-structured gold ran out (PI: P. Schwerdtfeger; NZ\$ 630,000 over three years). Behnam Assadollahzadeh worked on this project as a PhD student, and he submitted his PhD thesis to the research office in December this year. One Marsden grant on parity violation effects in chiral molecules started in 2007 (NZ\$ 870,000 over three years). This grant was the third largest in the country, and the largest running for the group of P.S. at Massey University. This project represents one of the most important research areas for the next three years and involves extensive collaboration with three major research groups in France (Strasbourg, Rennes and Paris) and one in Amsterdam.

In 2007 our centre was able to secure four new major Marsden grants, which is unprecedented for a small centre like ours (!). In fact, our centre received more Marsden grants than the rest of IFS. In dollar terms, our centre received 82% of the Marsden funding of IFS within the PSE panel, and 39.5% of all Marsden funding within Massey University. This clearly demonstrates the excellence of science carried out here in Albany. The successful Marsden grant winners were Joachim Brand (Please don't stand in my way, Sir! Studying the few-particle dynamics of ultra-cold atoms, NZ\$ 670,000 over 3 years), Ulrich Zülicke (Jitterbug on a chip: semiconductor nanospintronics meets relativistic quantum physics, NZ\$ 800,000 over 3 years), Patrick Bowman (Bondage and Confinement: How Hadrons keep their Quarks, NZ\$ 170,000 over 2 years), and Peter Schwerdtfeger (Chemistry at extreme conditions: materials at ultra-high pressures from first principles quantum theoretical methods, NZ\$ 720,000 over 3 years).

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 computer ran without major down-time for the whole year. 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 3 years old and at the end of its intended lifetime. It was therefore a great relief to us that the BestGrid machine came on line, which is already running at 0% idle time. All standard software is already installed on the BestGrid. As a consequence of the increased computer power, the number of publications increased substantially

compared to the year before, and two students (Behnam and Brian) were able to finish their research projects in time (Behnam submitted his PhD thesis in December and Brian will submit his one very soon). 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 enhanced. Chris Messom at IIMS is therefore preparing a business case for a large compute cluster called Helix³.

All members of CTCP were involved in chemistry and physics lab 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. M. Lein was involved in lab-teaching at the 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 (together with M. Lein) of *Introduction to Quantum Theory* for the year 3 Materials course. U. Zülicke taught physics papers in Palmerston North at all levels (stage 1 through to postgraduate, a total of 78 lectures + 18 tutorials).

Other activities: P. Bowman served on the IFS IT Committee. J. Brand served on the IFS Research and Equipment Committee. U. Zülicke served on the IFS Programmes Committee. P. Schwerdtfeger was chair of the IFS Research and Equipment Committee, and member of the IFS Management Committee and the Albany Academic and Research Advisory Committee. He also 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 is member of 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*.

Research Highlights: In collaboration with Florent Calvo (Lyon) we are simulating the melting behaviour of large rare gas clusters. Both E. Pahl and P. Schwerdtfeger visited Florent Calvo in France to discuss further collaborations. As a result of our visits, and some intensive programming work, we succeeded for the first time to be within 5 Kelvin of the experimental melting temperature of Argon, which has not been achieved so far. For the first time we were also able to explain the onset of optical absorption of water, which is blueshifted upon condensation and substantially opens the far-UV window. On the parity violation front we now investigate a very promising class of small but heavy chiral compounds; this class of molecules is not only theoretically accessible, but possibly experimentally as well. In addition, with the arrival of the BestGrid cluster, medium sized organometallic molecules with ~20 atoms are now investigated in our centre.

In collaboration with Rodrigo Vicencio from Chile and Sergej Flach from MIPPKS Dresden J. Brand predicted a novel type of resonance in the scattering of a cold atomic beam on a localized Bose-Einstein condensate kept in an optical lattice. The effect relies on a delicate interference effect among atoms interacting coherently with the localized matter wave. The work was published earlier this year in *Physical Review Letters* and received a lot of attention at international meetings such as the Quantum Gases Programme, a gathering of elite scholars including 4 Nobel laureates in Paris, and the conference Quantum Optics Downunder in Wollongong, Australia, where the results were presented.

Future opportunities and directions: The double-helix supercomputer at Albany is hopefully being upgraded in 2008. We aim for a Shared/Distributed (4x32, 8x16, 16x8) Parallel Compute Cluster which consists of 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) and 16 Distributed Units of 8 Shared Cores with a total of 128 Cores (32 quad-core processors). These will form a Compute Parallel Cluster. These systems will be 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 16GB of RAM (2GB RAM per

core). Each node will contain 1 small partition for the operating system and 4 x 1 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 requires urgently air-conditioning as the working environment in summer becomes unbearable in the huts occupied. Last year 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 with each unit producing 0.5 kWh in heat. We also need more space for the additional postdoctoral workers and PhD students joining our centre.

Invitations to a number of conferences for 2008 were received and some already accepted.

In 2008 we will join the newly established New Zealand Institute for Advanced Study (IAS), headed by Prof. Gaven Martin.

Performance against objectives: All objectives were met as we are a very productive research centre, with truly outstanding performances by each staff member at the international level. All papers published are in highly acclaimed journals of high impact factor. Four Marsden grants, one ISAT and one Dumont D'Urville grant were received in 2007.

In summary, it was a great year for our centre. This is also my last year as Deputy Director of IFS as I am moving into the IAS, and I personally like to thank all staff and students for their tremendous work and continuous support over the whole year. I believe that in comparing with other research centres in New Zealand, which are often bigger 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. Finally, my very special thanks goes to our Institute's secretary, Mrs. Vesna Davidovic-Alexander, who has helped us so much to run the centre, organizing conferences, looking after our visitors and many more.



Prof. Peter Schwerdtfeger

Date: December 20, 2007

Cc: Prof. Nigel Long (DVC)
Prof. P. Derrick (IFS)
Prof. G. Martin (IAS)

Appendix

Personnel

Prof. Peter Schwerdtfeger (Director of CTCP, Deputy Director of IFS)

Assoc. Prof. Joachim Brand (Deputy Director of CTCP)

Assoc. Prof. Uli Zülicke (based in Palmerston North)

Dr. Patrick Bowman (Lecturer)

Dr. Matthias Lein (Research Officer)

Honorary Research Fellows

Dr. Tilo Söhnel (Senior Lecturer, Auckland University)

Postdoctoral Fellows

Dr. Detlev Figgan (Marsden fellow, from February 1)

Dr. Elke Pahl

PhD Students

Behnam Assadollahzadeh

Susan Biering

Thomas Ernst

Andreas Hermann

Christian Thierfelder

Brian Vest

Exchange Students

Sacha Schäfer (TU Darmstadt)

Jonas Reuter (Bonn)

Secretary

Vesna Davidovic-Alexander

Visitors from other institutions:

Long Term:

Prof. Dietmar Kolb (University of Kassel, Germany, November 2006-April 2007)

Prof. Ian Hamilton (Wilfried Laurier University, Canada, December 2006 – June 2007)

Prof. Phil Bunker (NRC, Ottawa Canada, November 07–January 08)

Prof. Andrey Kolovsky (Academy of Sciences, Krasnayarsk, Russia, November 2007)

Short Term:

Howard Carmichael (Auckland)

Victor Flambaum (UNSW)

Debashis Gangopadhyay (S.N.Bose National Centre For Basic Sciences)

Tania Haigh (Massey PN)

David Hutchinson (Otago)

Piush Jain (Victoria)

Rudolf Kiefer (Auckland)

David Krofcheck (Auckland)

Alan O'Cais (Adelaide)

Cather Simpson (Auckland)

Tanja van Mourik (St. Andrews)

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
High-Pressure Physics
Quantum Chromodynamics
Relativistic Quantum Chemistry
Simulation of Bose-Einstein Condensates
Solid State Physics
Superheavy Elements
Theoretical Inorganic and Organic Chemistry
Theory of functional nanostructures; Spintronics

Grants Received/Continuing

- P. Bowman received a Marsden Fast-Start for the project "Bondage and Confinement: How Hadrons keep their Quarks" (NZ\$ 170,000).
- P. O. Bowman and J. Brand received a CEF grant over NZ\$60,000 for a 16 node computer for the project "Cluster for Cold Atoms."
- J. Brand received a Marsden grant of NZ\$ 670,000 over three years for the project "Please don't stand in my way, Sir! Studying the few-particle dynamics of ultra-cold atoms."
- J. Brand received grant from MU International Visitors Research Fund for the project "Transport of Cold Fermions" towards funding the visit of Prof. A. Kolovsky.
- J. Brand received travel grants from Centre Emile Borel Paris (EUR 950), Max-Planck Society (EUR 1,500), Harvard-Smithsonian Center for Astrophysics (US\$ 850).
- A. Hermann received a NZ International Doctoral Scholarship by Education New Zealand (starting January 2007) NZ\$ 18,000 per year for 3 years.
- E. Pahl and P. Schwerdtfeger received a Dumont D'Urville scholarship to visit Florent Calvo in Lyon (NZ\$ 3,900).
- P. Schwerdtfeger received an extension of the Marsden grant for the project "Nanostructures of Gold – From Low-Dimensional Assemblies to Heterogeneous Catalysis" (2003-07), year 4, NZ\$ 210,000 per annum for 3 years.
- P. Schwerdtfeger received a Marsden grant for the project "The Search for Molecular Parity Violation - A Synergy between Theory and Experiment" (2007-09), which started in January 2007. NZ\$ 290,000 per annum for 3 years.
- P. Schwerdtfeger received a Marsden grant for the project "Chemistry at extreme conditions: materials at ultra-high pressures from first principles quantum theoretical methods", NZ\$ 720,000 over 3 years.
- P. Schwerdtfeger received NZ\$ 2,700 from the ISAT linkage Fund to visit the University of Stuttgart.
- P. Schwerdtfeger received funding from Massey University for three long-term international visitors (NZ\$ 3,800 per visitor).
- U. Zülicke received a Marsden grant for the project "Jitterbug on a chip: semiconductor nanospintronics meets relativistic quantum physics", NZ\$ 800,000 over 3 years.
- U. Zülicke received EUR 8,000 support during his position as Visiting Professor at the Centre for Functional Nanostructures, University of Karlsruhe, Germany.
- U. Zülicke is a Partner Investigator on two successful ARC grant applications: Discovery project "Nanospintronics - Spin transport in semiconductor nanostructures" (AU\$ 380,000 for 3 years) and Linkage project "Nanoscale electronic devices: Bringing sample design, fabrication, test and theory together" (AU\$ 80,000 for 3 years).

Awards

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.

Thomas Ernst (PhD thesis): *Time dependent many-body theory for degenerate quantum gases.* Supervisor: J. Brand.

Lectures at Conferences / Meetings

P. Bowman

- Contributed talk given at NZIP Conference, Dunedin, July 2007: "How do hadrons keep their quarks?"

A. Hermann

- Invited talk at the Mathematical & Computational Nanoscience '07 meeting in Wellington, December 12: "Calculating water's optical spectrum: many-body effects, electrostatics, and coordination."

J. Brand

- Invited lecture at the international seminar and workshop Nonlinear Physics in Periodic Structures and Metamaterials (NPPSM07), Dresden, Germany, March 2007: "Nonlinear Quantum Physics with Bose-Einstein Condensates – Localization by Entanglement."
- Invited talk at NPPSM07: "Fano Blockade by a Bose-Einstein Condensate in an Optical Lattice."
- Invited talk at ITAMP workshop (Harvard-Smithsonian Center for Astrophysics) on Quantum Reflection, Cambridge MA, October 2007: "Quantum Reflection of Matter-Wave Solitons from Potential Wells."
- Contributed talk at NZIP conference, Dunedin, July 2007: "Localization of Matter Waves by Nonlinearity and Entanglement".
- Contributed talk at the Biannual meeting of the Australian Association of von-Humboldt fellows, Melbourne, September 2007: "Solitons in Bose-Einstein condensates – old wave phenomena in new disguises."
- Contributed talk at Quantum Atom Optics, OSA topical meeting, Wollongong, Australia, December 2007: "Fano Resonances and Quantum Localization of a Bose-Einstein condensate in an optical lattice."

E. Pahl

- Invited talk at the Mathematical & Computational Nanoscience '07 meeting in Wellington, December 12: "Melting of Nanoclusters."
- Contributed talk at the 'International Workshop on Local Correlation Methods: From Molecules to Clusters' at the MPIPES, Dresden, September 12-15, Title: "Calculation of band structures using wave-function based correlation methods".

P. Schwerdtfeger

- Invited talk at the Mathematical & Computational Nanoscience '07 meeting in Wellington, December 12: "Towards the Simulation of Mercury Clusters."
- Plenary Talk at the Relativistic Effects in Heavy Elements (REHE) 2007 Conference, Ottrott, France, on "Relativistic Effects in the Solid State", March 23.
- Keynote lecture at the Computational Actinide and Transactinide Chemistry, Nuclear Chemistry Subdivision, ACS Boston Meeting, Boston, August 21, 2007, on "The Chemistry of Superheavy Elements".
- Invited Lecture at the 12th Biennial Meeting, Australian Catholic University (St Patrick's Campus) Fitzroy, Victoria, Australia, September 8, 2007, on "Kepler's Conjecture, Newton's Kissing Problems and How to Pack Rare Gas Atoms."
- Keynote lecture at the TAN07- International Conference on Transactinide Chemistry, Davos, September 27, 2007, on "Four Component Relativistic Calculations for Transactinide Elements and Their Compounds."
- Keynote lecture at the Stuttgarter Chemietage, Institut Dr. Flad, Stuttgart, September 26-29, 2007, on "Albert Einstein and Chemistry – A Useful Symbiosis."
- Invited lecture at the Mathematical and Computational Nanoscience 3007, MacDiarmid Institute, Wellington, December 9-11, 2007, on "Towards the Accurate Simulation of Mercury Clusters."

U. Zülicke

- Invited talk at the Mathematical & Computational Nanoscience '07 meeting in Wellington, December 11: "Spin and pseudospin effects in quantum-confined systems."
- Invited talk at the SPIE conference on Microelectronics, MEMS, and Nanotechnology, Canberra, Australia, December 5: "Engineering of hole-spin polarization in nanowires."
- Plenary talk at the Trends in Nanotechnology (TNT2007) Conference, San Sebastian, Spain, September 4: "Nanospintronics meets relativistic quantum physics: Ubiquity of Zitterbewegung effects."
- Invited talk, Final Colloquium of DFG Main Focus Programme Quantum Hall Systems, Hannover, Germany, June 30: "Andreev edge states: Recent results, new experiments, and possible applications."
- Contributed talk, 3rd International Conference on Advanced Materials and Nanotechnology (AMN-3), Wellington, New Zealand, February 16: "Electronic and spin properties of hole point contact."
- Contributed talk, AMN-3 Satellite Meeting on Nano- & Bionano-Technology, Quantum Transport in Synthetic Metals and Quantum Functional Semiconductors (NBT-QT2007), Wellington, New Zealand, February 9: "Spin splitting in hole nanowires."

Seminars

- J. Brand gave a Physics Colloquium talk at Melbourne University, September 2007 on "Solitons and Vortices in Bose-Einstein Condensates" and seminars at Chemnitz University of Technology (January 2007): "Solitons in Bose-Einstein condensates"; Max Planck Institute for the Physics of Complex Systems, Dresden (March 2007): "Solitons in Bose-Einstein condensates"; Heidelberg University (April 2007): "Solitons, Fano Blockade, and quantum localization with ultra-cold atoms"; Institute Henri Poincaré, Paris (May 2007): "Fano Resonances in Atom Scattering on a Bose-Einstein Condensate"; Massey University Palmerston North (November 2007): "Fano resonances and quantum localization."
- P. Bowman gave talks on "Gross Properties of QCD: Chiral Symmetry Breaking and Confinement" at the University of Auckland, Physics Department, October 2007; and on "On the structure of matter: It's mostly glue" at Massey University, Auckland, IFS, September 2007.

- A. Hermann, BioNano Meeting, Massey University PN on “Calculating water's optical spectrum: many-body effects, electrostatics, and coordination”, October 26.
- M. Lein, BioNano Meeting, Massey University PN on “Carbon-Monoxide on Gold Surfaces - harder than expected”, October 26.
- E. Pahl, BioNano Meeting, Massey University PN on “Melting of Nanoclusters”, October 26.
- P. Schwerdtfeger gave talks at the Einstein University of Ulm (January 9, Title: The Quest for Absolute Chirality); the Georg-August Universität Göttingen (January 18, Title: The Chemistry and Physics of the Superheavy Elements); University of Stuttgart (January 23, Title: Relativistic Effects in the Solid-State); Massey University, IFS Albany (February 23, Title: The Pseudopotential Approximation); Massey University PN (March 13, Title: The Origin of Biomolecular Homochirality); Massey University College of Science Seminar (Superheavy Elements, March 15,); Chemistry Department, University of Queensland (April 10, Title: The Quest for Absolute Chirality); Physics Department, Griffith University (April 11, Title: Kepler's Conjecture, Newton's Kissing Problems and How to Pack Rare Gas Atoms); Chemistry Department, Charles Darwin University (April 13, Title: The Chemistry and Physics of the Superheavy Elements); Chemistry Department, The University of New South Wales (April 17, Title: The Quest for Absolute Chirality); Chemistry Department, Sydney University (April 18, Title: Relativistic Effects in the Chemistry of Gold); Physics Department, The University of New South Wales (April 18, Title: Small effects, large consequences: from relativity to electroweak interactions); Research School of Chemistry, The Australian National University (April 20, Title: The Quest for Absolute Chirality); Chemistry, Otago University, IFS Albany (May 4, Title: The Pseudopotential Approximation); Physics, Otago University (May 7, Title: Parity Violation in Molecules); Chemistry, Canterbury University, IFS Albany (May 8, Title: The Chemistry and Physics of the Superheavy Elements); Laboratoire de Physique Quantique, Université Paul Sabatier (June 5, Title: Simulation of Mercury Clusters; and June 6, Title: The Quest for Absolute Chirality); Chemistry Department, Victoria University Wellington (August 7, Title: The Quest for Absolute Chirality); Chemistry Department, Waikato University Hamilton (August 17, Title: The Quest for Absolute Chirality); Chemistry Department, The University of Western Australia (August 31, Title: Relativistic Effects in the Chemistry of Gold); Chemistry Department, University of Adelaide (September 3, Title: The Chemistry and Physics of the Superheavy Elements); Chemistry Department, University of Tasmania (September 5, Title: The Chemistry and Physics of the Superheavy Elements); Physics Department, University of Tasmania (September 5, Title: Kepler's Conjecture, Newton's Kissing Problems and How to Pack Rare Gas Atoms); Chemistry Department, Monash University (September 10, Title: The Chemistry and Physics of the Superheavy Elements); Chemistry, RMIT Melbourne (September 12, Title: The Quest for Absolute Chirality); Paul-Scherrer Institut, Villigen, Switzerland (October 2, Title: The Quest for Absolute Chirality); Chemistry Department, Universität Bern (October 3, Title: Kepler's Conjecture, Newton's Kissing Problems and How to Pack Rare Gas Atoms); Physics Department, Heinrich-Heine Universität Düsseldorf (October 5, Title: Parity Violation Effects in Molecules); Philipps Universität Marburg (October 9, Title: Relativistic Effects in the Solid-State); BioNano Meeting Massey University PN (October 26, Title: Simulation of Mercury Clusters); Chemistry Department, University of Auckland (November 15, Title: Left or Right in Nature, That is the Question).
- U. Zülicke gave invited seminar talks on “Nanospintronics meets relativistic quantum physics: Ubiquity of Zitterbewegung effects” at the Centre for Functional Nanostructures, University of Karlsruhe, Germany (June 18), the Department of Physics, Ruhr-University

Bochum, Germany (July 4), and the Department of Physics, University of Regensburg, Germany (July 12); and on “*Zitterbewegung* and magnetic focusing of charge carriers from spin-split bands” at the Division of Solid-State Physics, Lund University, Sweden (June 11).

Posters

A. Hermann

13th International Conference on Surface Science (ICSS-13), Stockholm, July. Authors: A. Hermann, W. G. Schmidt, P. Schwerdtfeger, Title: "Theoretical study of the localization of excess electrons at the surface of ice."

Th. Ernst

- Th. Ernst and J. Brand “Trapping of matter-wave solitons in a quantum well” presented at ACQAO summer school at Kioloa, Australia and at the OSA topical meeting Quantum-Atom Optics down-under, Wollongong, Australia, December 2007

U. Zülicke

- U. Zülicke, “Novel dynamics in spin-split bands: *Zitterbewegung* and magnetic focusing”, presented at 2007 Winter Conference on Condensed Matter, Aspen Center for Physics, Aspen, Colorado, USA, January 2007.

P. Schwerdtfeger

P. Schwerdtfeger, “The Packing of Rare Gas Atoms”, International Conference in Honour of Professor Peter Pulay, Molecular Quantum Mechanics - Analytic Gradients and Beyond, May 29 - June 3, 2007.

Other activities

Papers refereed:

- P. Bowman refereed papers for Physical Review D and Physical Review Letters.
- J. Brand refereed papers for J. Phys. B, J. Phys. Cond. Matt., Physica A, Phys. Rev. A, Phys. Rev. Lett., Europhys. Lett. He also refereed a grant proposal for Binational Science Foundation (US Israel).
- M. Lein is regular referee for the Journal of Computational Chemistry, Coordination Chemistry Reviews and J. Mol. Struct. (Theochem).
- P. Schwerdtfeger refereed 73 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. Mol. Struct. (Theochem.) and many more.
- U. Zülicke is a regular referee for Physical Review Letters, Physical Review B, Europhysics Letters, Applied Physics Letters, New Journal of Physics, and Physica E. He has also refereed one grant proposal for the US National Science Foundation and three Discovery-project grant proposals for the Australian Research Council.

Community Outreach:

PhD and MSc theses refereed:

- J. Brand refereed one PhD thesis from the Australian National University
- J. Brand refereed one MSc thesis from the University of Auckland
- J. Brand refereed a physics textbook for Cengage learning.
- U. Zülicke examined a PhD thesis from the University of New South Wales.

Chairs at Conferences

- P. Schwerdtfeger chaired session at the Relativistic Effects in Heavy Elements (REHE) 2007 Conference, Ottrott, France, March 21-25; at the International Conference in Honour of Professor Peter Pulay, Molecular Quantum Mechanics - Analytic Gradients and Beyond, May 29 - June 3, 2007; at TAN07- International Conference on Transactinide Chemistry, Davos, September 23-28, 2007 (K).

PUBLISHED WORK

Papers published in refereed journals

1. P. O. Bowman, U. M. Heller, D. B. Leinweber, M. B. Parappilly, A. Sternbeck, L. von Smekal, A. G. Williams, J. Zhang, "Scaling behavior and positivity violation of the gluon propagator in full QCD", *Phys. Rev. D* 76, 094505-1-7 (2007).
2. J. Brand, A. R. Kolovsky, "Emergence of superfluid transport in a dynamical system of ultra-cold atoms", *Europhys. J. D* 41, 331-336 (2007).
3. D. Csontos, and U. Zülicke, "Large variations in the hole spin splitting of quantum-wire subband edges", *Phys. Rev. B* 76, 073313-1-4 (2007).
4. N. Gaston, I. Opahle, H. W. Gäggeler, P. Schwerdtfeger, "Is Eka-Mercury (Element 112) a Group 12 Metal?", *Angew. Chem. Int. Ed.* 46, 1663-1666 (2007). *Angew. Chem.* 119, 1692-1695 (2007).
5. E. Goll, H. Stoll, C. Thierfelder, P. Schwerdtfeger, "Improved dipole moments from coupling short-range gradient-corrected density functional with long-range wave-function based theory", *Phys. Rev. A* 76, 032507-1-7 (2007).
6. A. Hermann, M. Lein, P. Schwerdtfeger, "The Gregory-Newton Problem of Kissing Sphere Applied to Chemistry: The Search for the Species with the Highest Coordination Number.", *Angew. Chem. Int. Ed.* 46, 2444-2447 (2007). *Angew. Chem.* 119, 2496-2499 (2007).
7. A. Hermann, R. P. Krawczyk, M. Lein, P. Schwerdtfeger, I. P. Hamilton, J. J. P. Stewart, "Convergence of the many-body expansion of interaction potentials: From van der Waals to covalent and metallic systems", *Phys. Rev. A* 76, 013202-1-10 (2007).
8. S. Heislbetz, Peter Schwerdtfeger, G. Rauhut, "Vibrational Spectra Obtained from High Quality Potential Energy Surfaces Spanned by Low Level Normal Coordinates - Application to CHFCl and CDFCl", *Mol. Phys.* 105, 1385-1394 (2007).
9. C. R. Jacob, L. Visscher, C. Thierfelder, P. Schwerdtfeger, "Nuclear quadrupole moment of ^{139}La from relativistic electronic structure calculations of the electric field gradients in LaF, LaCl, LaBr and LaI ", *J. Chem. Phys.* 127, 204303-1-7 (2007).
10. S. Johnson, U. Zülicke, A. Markwitz, "Universal characteristics of resonant-tunneling field emission from nanostructured surfaces", *J. App. Phys.* 101, 123712-1-5 (2007).
11. W. Kamleh, P.O. Bowman, D.B. Leinweber, A.G. Williams, J.B. Zhang, "Unquenching effects in the quark and gluon propagator", *Phys. Rev. D* 76, 094501-1-9 (2007).
12. M. Lein, A. Hammerl, H. L. Hermann, P. Schwerdtfeger, "Theoretical Investigations into Trioxo Group 7 Compounds LRO_3 with Perfluorated Ligands (M = Mn, Tc, Re; R = F, CF_3 , C_3F_5 , and C_6F_5)", *Polyhedron* 26, 486-492 (2007). (invited paper)
13. I. S. Lim, P. Botschwina, R. Oswald, V. Barone, H. Stoll, P. Schwerdtfeger, "Calculated spectroscopic and electric properties of the alkali metal-ammonia complexes from $\text{K}^n\text{-NH}_3$ to $\text{Fr}^n\text{-NH}_3$ ($n = 0, +1$)", *J. Chem. Phys.* 127, 104313-1-12 (2007).

14. G. E. Moyano, P. Schwerdtfeger, K. Rosciszewski, "Lattice dynamics from *ab initio* potentials for the fcc rare gas solids Ne, Ar, and Kr", *Phys. Rev. B* 75, 024101-1-6 (2007).
15. S. Schäfer, M. Mehring, R. Schäfer, P. Schwerdtfeger, "Polarizabilities of Ba and Ba₂: Comparison of molecular beam experiments with relativistic quantum chemistry", *Phys. Rev. A* 76, 052515-1-5 (2007).
16. P. Schwerdtfeger, "Back to the Basics", *ChemNZ. July issue*, 50-52 (2007).
17. C. Thierfelder, P. Schwerdtfeger, T. Saue, " ⁶³Cu and ¹⁹⁷Au Nuclear Quadrupole Moments from Four-Component Relativistic Density Functional Calculations using Exact Long-Range Exchange", *Phys. Rev. A* 76, 034502-1-4 (2007).
18. C. Thierfelder, W. G. Schmidt, "Ethanol adsorbed on ice: A first-principles study", *Phys. Rev. B* 76, 195426-1-5 (2007).
19. R. A. Vicencio, J. Brand, S. Flach, "Fano Blockade by a Bose-Einstein Condensate in an Optical Lattice", *Phys. Rev. Lett.* 98, 184102-1-4 (2007).
20. R. Winkler, U. Zülicke, J. Bolte, "Oscillatory multiband dynamics of free particles: The ubiquity of zitterbewegung effects", *Phys. Rev. B* 75, 205314-1-10 (2007).
21. U. Zülicke, J. Bolte, R. Winkler, "Magnetic focusing of charge carriers from spin-split bands: semiclassics of a Zitterbewegung effect", *New J. Phys.* 9, 355-1-14 (2007). (invited paper)
22. U. Zülicke, A. I. Signal, "Rashba interferometers: Spin-dependent single and two-electron interference", *Solid St. Commun.* 144, 529-535 (2007). (invited paper)

Conference Proceedings

23. R. Danneau, O. Klochan, W. R. Clarke, L. H. Ho, A. P. Micolich, M. Y. Simmons, A. R. Hamilton, M. Pepper, D. A. Ritchie, U. Zülicke, "Anisotropic Zeeman splitting in ballistic one-dimensional hole systems", *AIP Conference Proceedings* 893, 699-700 (2007).

Book chapters:

24. J. Brand, L. D. Carr, and B. P. Anderson in "Emergent Nonlinear Phenomena in Bose-Einstein Condensates", eds. P. G. Kevrekidis, D. J. Frantzeskakis, and R. Carretero-Gonzales, Springer Heidelberg, 2008, ISBN: 978-3-540-73590-8.
25. L. D. Carr and J. Brand in "Emergent Nonlinear Phenomena in Bose-Einstein Condensates", eds. P. G. Kevrekidis, D. J. Frantzeskakis, and R. Carretero-Gonzales, Springer Heidelberg, 2008, ISBN: 978-3-540-73590-8.