

**CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
NEW ZEALAND INSTITUTE FOR ADVANCED STUDY,
INSTITUTE OF NATURAL SCIENCES
and INSTITUTE OF FUNDAMENTAL SCIENCES**

Bldg. 40 and 44, Private Bag 102 904, North Shore MSC, Auckland, New Zealand

Ph: +64-9-4140800 ext. 9780, FAX: +64-9-443 9779

Email: p.a.schwerdtfeger@massey.ac.nz, Web: <http://ctcp.massey.ac.nz>

2010 REPORT TO UNIVERSITY COMMERCIAL ACTIVITIES GROUP (CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS)

Objectives of Research Centre: *Our objective is to advance and disseminate knowledge in the area of theoretical chemistry and physics, and to maintain high international standards in this research field.* All objectives were clearly met as we are (to our knowledge) the most productive research centre 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 such as *Angewandte Chemie* or *Physical Reviews*. I believe that, compared with other research centres in New Zealand – which are often much larger in size than ours with much greater research funding – we have achieved a very high international standing. This again is reflected by the many invitations to present keynote and plenary lectures overseas, the funding of postdoctoral fellows by overseas agencies (mainly DAAD and Humboldt Foundation), the 6 Marsden grants currently running in our centre, the many high-standing international visitors who joined our research centre this year, the promotion of Joachim Brand to the professorial level, and the award of a major international research prize (the Humboldt Research Award) to Peter Schwerdtfeger.

Research Output: This year we published 40 papers amongst 5 academic staff in top journals, a truly exceptional year for our research centre. See attached list of publications for details.

Activities and achievements: All members of CTCP were involved in chemistry and physics teaching as outlined in the appendix. Almost all postdoctoral fellows helped in lab teaching at stage 1 level. Notable achievements are the promotion of Dr. Joachim Brand to the professorial level, Dr. Patrick Bowman to the Senior Lecturer Level, the appointment of Elke Pahl to the Lecturer level, the election of Uli Zülicke to Fellow of the New Zealand Institute of Physics, and the Humboldt Research Prize for the Director of CTCP.

The Future – Opportunities, Risks and Directions: The Double-Helix Computer Cluster was purchased in 2004 with up to ten times the computational power of the university's existing supercomputer, the 64-node Helix 1 as a replacement for the Helix-1 supercomputer. This year we saw all remaining nodes failing but we were able to gradually replace half of the nodes by new pieces of equipment. An insurance claim of 40,000 NZ\$ for damage of equipment due to a power-cut in Albany was processed successfully. We also applied to the Massey University capital equipment expenditure fund to replace all remaining original compute nodes.

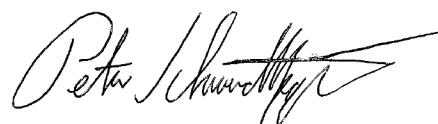
The computer room in Albany still requires a power back-up generator, but nothing has been done to address this problem. We pointed out last year that in financial terms, the damage caused by the recent power cut is larger than the cost would have been for the purchase of such a power generator. Another drawback is the limited access to international journals through our less well-equipped library. We are clearly an *internationally focused* (!) research centre, with strong national and international reputation, requiring the support of an internationally well recognized and equipped University.

Work in progress: There are too many research projects in progress to list all of them. See attachment for more details. Funding in 2011 is anticipated through additional Marsden Grants and a Dumont d'Urville research programme together with the University of Lyon. Further, being the campus of innovation (and certainly excellence as well), the chemistry group is planning to move into environmental sciences, addressing issues like the Pike-Mine accident and global warming, by designing efficient methods for gas separation and storage.

Staffing: In 2010 we saw staff leaving and new ones coming on board. Dr. Matthias Lein left our research centre to take up a position at Senior Lecturer level at Victoria University. Matthias has served our centre for many years. He has contributed to our centre immensely and will be truly missed. We wish him all the best for his future career at Victoria University. His interim replacement will be Dr. James Avery from Copenhagen. Dr. Detlev Figgen's Marsden postdoctoral fellowship finished. His activities were rewarded with a cover page for *Angewandte Chemie*. Dr. Michael Wormit started on a Feodor-Lynen fellowship of the German Alexander von Humboldt Foundation as post-doctoral fellow (2 years of funding). Dr. Jonas Wiebke started on a DAAD fellowship (2 years funding). Dr. Andreas Hauser from Graz University started as a postdoctoral fellow working on methane separation. Dr. Oleksandr Fialko started on a Marsden postdoctoral fellowship. And finally, Mustafa Hasanbulli, having been already awarded one PhD in North Cyprus, started for his second one in the area of Mathematical Physics in our research centre. For further information see the attachment.

Financial: See attachment

Other comments: We enjoyed constant moral and financial support from Nigel Long, Robert Anderson and Gaven Martin. We also thank Mustafa Hasanbulli for the wonderful design of our new centre logo. 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 our research centre, organizing conferences and meetings, looking after our demanding overseas visitors, and organizing us as well (to some success).

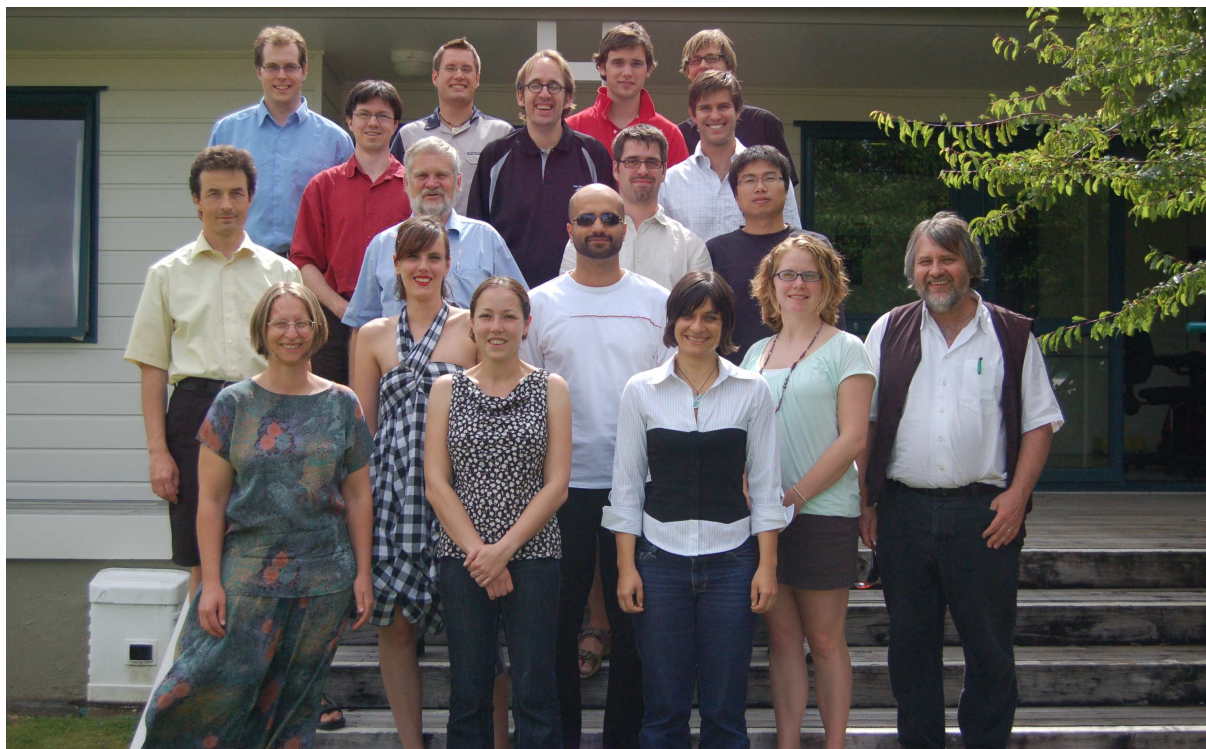


Prof. Peter Schwerdtfeger

Date: December 12, 2010

Cc: Hon. Steve Maharey (VC), Prof. Gaven Martin (Director, INS and IAS), Prof. Peter Derrick (Director, IFS)

Appendix



Our research centre (from the left to the right):

Joachim Brand, Matthias Lein, Elke Pahl, Patrick Bowman, Camilla Evangelisti, Heinz Gäggeler, Thomas Ernst, Anastasia Borschevsky, Detlev Figgen, Behnam Assadollahzadeh, Jake Gulliksen, Ralf Tonner, Susan Biering, Urban Rohrmann, David Hallwood, Renyuan Liao, Julie Coxe, Peter Schwerdtfeger.

Missing in this picture: Kyle Beloy, Andreas Hermann, Andreas Hauser, Jonas Wiebke, Michael Wormit, Mustafa Hasanbulli, Oleksandr Fialko, Andrew Punnet, Christian Thierfelder, Ulrich Zülicke (Palmerston North), Brian Vest, Vesna Davidovic-Alexander

Personnel:

Prof. Peter Schwerdtfeger (Director of CTCP)

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 until August 30, then Honorary Research Fellow)

Dr. Elke Pahl (Lecturer, from July 1, 2010)

Secretaries:

Vesna Davidovic-Alexander (IAS)

Muharram Khoussainova (INS)

PhD Students:

Susan Biering

Thomas Ernst

Mustafa Hasanbulli (since October 2010)

Christian Thierfelder

Andrew Punnett

MSc Students:

Julie Coxé

Jake Gulliksen

Exchange Students:

Urban Rohrmann (Darmstadt)

Postdoctoral Fellows:

Dr. Behnam Assadollahzadeh (Marsden fellow)

Dr. Kyle Beloy (Marsden fellow)

Dr. Anastasia Borschevsky (Marsden fellow)

Dr. Oleksandr Fialko (Marsden fellow)

Dr. Detlev Figgen (Marsden fellow, until March 31, 2010)

Dr. Andreas Hauser (Postdoctoral Fellow, since September 2010)

Dr. Renyuan Liao (Massey postdoctoral fellow)

Dr. David Hallwood (Marsden fellow)

Dr. Andreas Hermann (Honorary research fellow)

Dr. Elke Pahl (until June 30, 2010)

Dr. Ralf Tonner (Alexander von Humboldt Feodor Lynen fellow,
until February 2010, now University of Marburg/Germany)

Dr. Michael Wormit (Alexander von Humboldt Feodor Lynen fellow, since June 2010)

Dr. Jonas Wiebke (DAAD Fellow, since November 2010)

Visitors from other institutions:

Long Term:

Prof. Phil Bunker (NRC, Ottawa Canada)

Dr. Florent Calvo (University of Lyon)

Dr. Alexander Cherny (Joint Institute for Nuclear Research, Dubna)

Prof. Victor Flambaum (University of New South Wales)

Prof. Heinz Gaggeler (Bern University and PSI Villigen)

Dr. Mirian Tsulaia (University of Liverpool).

Short Term:

Dr. Ashton Bradley (University of Otago)

A/Prof. Blair Blakie (University of Otago)

Dr. Simon Gardiner (University of Durham)

Prof. D. Goldschnigg (Graz University)

Prof. S. Hashmi (Heidelberg University)

Prof. Günther Radons (Chemnitz University of Technology)

Prof. H. Schwarz (President of the Humboldt Foundation, TU Berlin)

Dr. Cedric Simenel (ANU, Canberra)

Current Research Activities:

Adsorption of organic molecules on semi-conductor surfaces

Cluster Simulations and Phase Transitions, Nanoscience

Density Functional and Ab-initio Theory

Frequency shifts in atomic clocks

Electroweak Electronic Structure Theory

Heterogeneous and Homogeneous Catalysis

High-Pressure Physics

Macroscopic quantum superpositions

Nonlinear waves in Bose-Einstein Condensates

Nonperturbative QED
 One-dimensional quantum fluids
 Quantum Chromodynamics
 Quantum dynamics of ultra-cold few-atom systems
 Relativistic Quantum Chemistry
 Solid State Physics
 Spin-dependent parity violation in diatomic molecules
 Strongly-correlated fermionic superfluids
 Superheavy Elements
 Surface enhanced Raman spectroscopy
 Theoretical Inorganic and Organic Chemistry
 Theory of functional nanostructures; Spintronics
 Transition Metal Catalysis and Theory of Chemical Bonding
 Variation of Fundamental Constants in Space-Time

Grants Received/Continuing:

- J. Brand is in his final year of 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 (MAU0706). He continues on one other Marsden grant as principal investigator (09MAU048) on "*Icy tornadoes in the quantum world – Josephson junctions of Bose-Einstein condensates*" started in 2010 (NZ\$ 785,000).
- A. Hermann received a personal postdoctoral fellowship by the New Zealand Foundation for Research, Science and Technology for the project "Modelling liquid transport through nanopores", to be run together with Dr. S. Hendy from Victoria University Wellington.
- E. Pahl and P. Schwerdtfeger are continuing on a Dumont D'Urville scholarship received in 2009 together with F. Calvo (Lyon).
- P. Schwerdtfeger is in his second year 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 one other Marsden grant as principal investigator, "*Chemistry at extreme conditions: materials at ultra-high pressures from first principles quantum theoretical methods*", NZ\$ 240,000 per annum, third and final year of funding (07MAU016). He also received Euro 40,000 grant in aid from the Alexander von Humboldt Foundation to run the conference on "In the Spirit of Alexander von Humboldt and Friedrich von Humboldt: The Role of Fundamental Research in our Society." In Dunedin, January 28-30, 2010.
- U. Zülicke continues on a Marsden grant "*Jitterbug on a chip: Semiconductor nanospintronics meets relativistic quantum physics*" (awarded 2007, contract MAU0702), and continues his AI role in Joachim's Marsden grant "*Icy tornadoes in the quantum world*" (awarded 2009).

Honours and Awards:

- S. Biering was awarded first prize for her poster with the title "*The influence of relativistic effects on the structure of the group 12 chalcogenides: A density functional study*" in the poster competition at the 34th Annual Condensed Matter and Materials meeting (02-05.02.10, Waiheke, Auckland).
- P. Schwerdtfeger received the 2010 Humboldt Research Prize. The international award valued at 60,000 Euros is granted in recognition of a researcher's entire achievements to date. It is awarded to academics whose fundamental discoveries, new theories, or insights have had a significant impact on their own discipline and who are expected to continue producing cutting-edge achievements in the future.
- U. Zülicke was elected Fellow of the New Zealand Institute of Physics.

Ongoing MSc Theses:

- J. Gulliksen: *Few-atom dynamics in a double-well potential*. Supervisor: J. Brand.

Finished MSc Theses:

- J. Cox: *Squeezing Atoms Using a Confinement Potential*. Supervisor: P. Schwerdtfeger.

Ongoing PhD Theses:

- T. Ernst: *Time dependent many-body theory for degenerate quantum gases*. Supervisor: J. Brand.
- M. Hasanbuli: *Atoms in Spherical Confinements*. Supervisor: P. Schwerdtfeger and B. Pavlov (started October 15).
- A. Punnett: *How Hadrons keep their Quarks*. Supervisor: P. Bowman.

Finished PhD Theses:

- S. Biering: *The unusual structure of the mercury chalcogenides: relativistic effects in the solid state*. Thesis was handed in September 2010. Supervisor: P. Schwerdtfeger.
- C. Thierfelder: *Applications to the Dirac equation – from relativistic effects to electroweak interactions*. Thesis was handed in October 2009. Supervisor: P. Schwerdtfeger.

Lectures at Conferences / Meetings:

- S. Biering and T. Ernst participated at the Massey University 3 Minute Thesis Competition (21.04.2010), introducing their thesis topic and its significance to a non-specialist audience.
- A. Borschevsky: Talk at the ICAP conference in Cairns, Australia (25-30 July 2010): “Enhanced Sensitivity to Variation of the Fine Structure Constant and m_p/m_e in SiBr”.
- J. Brand gave invited talks at the Dodd-Walls Symposium (2 February) in Wellington, at the conference Nonlinearwave 2010 (27 June) in Beijing, China “Spectroscopy of bound states with matter-wave solitons”, at the conference Laser Physics 2010 (July 9) in Iguacu, Brazil, “Rotational Schrödinger Cats with Strongly-Correlated Ultra-Cold Atoms”, and at the International Symposium on Quantum Dynamics of Ultracold Atoms and Quantum Technology (8 December) in Guangzhou, China “Dark Solitary Waves and Robust Superpositions with Strongly Correlated Ultra-Cold Atoms”.
- D. Figgen presented a talk at the Humboldt Meeting in Dunedin (January 28-30): “Parity violation: Why enantiomers differ in energy and how to prove it”.
- D. Hallwood presented a talk at the 4th Annual Dodd-Walls Symposium in Wellington (31st January -3rd February 2010): “Robust mesoscopic quantum superpositions”.
- E. Pahl gave a talk at the 34th Annual Condensed Matter and Materials Meeting on Waiheke Island (2010) “Towards accurate melting temperatures from ab initio Monte Carlo simulations: from nano clusters to the bulk” and an invited talk at the Cluster Day, Marlborough Sounds (2010) “Towards the simulation of mercury”.
- P. Schwerdtfeger delivered the following keynote/plenary lectures: “High Pressure Simulations – Squeezing the Hell out of Atoms” at the Wagga-Wagga Solid State meeting, Waiheke Island, Auckland, February 2-5; the same talk at the 50th Sanibel Symposium, Brunswick (USA), February 24 - March 2; “The role of fundamental sciences in our society”, at the DAAD Conference on “Bridging the Distance – New Zealand and Germany in Dialogue”, Auckland, March 20-21; “The Accuracy of the Pseudopotential Application” at the 17th Canadian Conference on Theoretical Chemistry, Edmonton, Canada, July 25-30; “Bound State QED for Heavy Elements” at the REHE-2010 Conference on “Exact Relativistic Methods for Electronic Structure and Magnetic Property Calculations”, Beijing, China, September 25-29; “Relativistic CC calculations

for *PV effects in chiral molecules*” at the ICCMSE Conference in Kos (Greece), October 3-8; “*High Pressure Simulations – Squeezing the Hell out of Atoms*” at the MM2010 Conference in Melbourne, November 28-December 1; and two presentations at the PACIFICHEM Conference in Hawaii, December 15-20, title of the talks: “*Relativistic and quantum electrodynamic effects for the superheavy elements*” and “*The quest for absolute chirality*”.

- U. Zülicke: *Spin-dependent transport due to spin-orbit coupling*, 16 September (Lecture 1) and 18 September (Lecture 2), 2010 DPG School on Nano-Spintronics, Bad Honnef, Germany, 12 - 17 September 2010.

Seminars and Talks:

- A Borschevsky gave a seminar at the School of Chemistry, Tel Aviv University, Israel (14/10/2010). Topic: “*Variation of Fundamental Constants: Theory and Observation*”.
- J. Brand: J. Brand presented a talk at the conference Nonlinear Phenomena in Quantum Gases (14 April) in Ourense, Spain “*Dark Solitons in the Superfluid Fermi Gas*”. He gave a seminar at Tsinghua University (Beijing, 24 June) “*Robust Schrödinger cats with strongly correlated ultra-cold atoms*”.
- T. Ernst presented a talk at the Dodd-Walls Centre Student Conference in Dunedin in February this year.
- D. Hallwood visited and gave talks to physics groups in Heidelberg and Freiburg in Germany, and Durham in UK (3rd June - 25th June).
- A. Hermann gave a talk “*Solid state calculations of ice from an incremental coupled cluster approach*” at the Wagga2010 Solid State meeting, Auckland, February 2010; a talk “*Understanding water and ice: aqueous systems from first principles*” at the Graduiertenkolleg ‘Quantum and Gravitational Fields’ of the University Jena in Germany, July 2010; the same talk in the Chemistry Departmental Seminar Series, Auckland, November 2010; a talk “*Antifreeze Proteins: a computational perspective*” at the Cluster Day 2010 meeting, Marlborough, October 2010; and a guest lecture on the same topic in graduate level teaching in the Chemistry Department, Auckland, October 2010.
- E. Pahl gave a seminar on “*Melting of weakly-bound nano-clusters and extrapolation to the bulk system*”, Universidad Complutense de Madrid, Spain, May 2010.
- P. Schwerdtfeger gave a seminar on “*Bound State QED for Heavy Elements*” at Massey University, Albany, November 5.
- U. Zülicke gave a talk entitled *After the prize: Graphene continues to surprise*, 4 November 2010, MacDiarmid-Institute Videoconference Seminar involving Auckland U, Canterbury U, IRL, Massey U, Otago U, and Victoria U; on *Time reversal of a pseudospin: General properties and application to graphene*, 22 June 2010, Condensed Matter Physics Seminar, University of Science and Technology of China, Hefei, China; and on *Holes in nanowires and rings: Tuneable magnetic moments and enhanced spin-dependent interference*, 16 June 2010, Kavli Institute for Theoretical Physics China, Chinese Academy of Sciences, Beijing, China.

Posters:

- B. Assadollahzadeh presented a poster at the 34TH Annual Condensed Matter and Materials Meeting at Waiheke on “*The Global Minimum Structures and Corresponding Electronic Properties of Gold Clusters*”.
- K. Beloy presented two posters at the 22nd International Conference on Atomic Physics on “*Entangling the lattice clock: Towards Heisenberg-limited timekeeping*” and “*Improved test of the standard model of elementary particles with atomic parity violation*”.
- K. Beloy and A. Borschevsky presented a poster at the 22nd International Conference on Atomic Physics on “*Enhanced sensitivity to the time variation of fundamental constants in SiBr*”.

- S. Biering presented a poster titled "*The influence of relativistic effects on the structure of the group 12 chalcogenides: A density functional study*" at the 34th Annual Condensed Matter and Materials meeting (02-05.02.10, Waiheke, Auckland).
- A. Borschevsky and K. Beloy presented a poster at ICAP, Cairns, Australia (25-30 July 2010), on "*Enhanced Sensitivity to Variation of the Fine Structure Constant and m_p/m_e in SiBr*".
- T. Ernst presented a poster on "*Full quantum behaviour of ultracold atoms*" at the annual Dodd-Walls Symposium in Wellington, February 2010. He also presented a poster with the same title but different content at the KOALA student conference in Dunedin, December 2010.

Teaching:

- P. Bowman taught parts of 124.101 and 124.102, stage 1 physics, and was paper coordinator for new paper 124.129 Astronomy.
- J. Brand taught parts of 124.101 and 124.102, stage 1 physics and part of 124.129 Astronomy.
- M. Lein taught parts of 124.101 (Lab course, chemistry) and 123.102 (Lectures, Physics). as well as parts of CHEM302 (advanced spectroscopy), CHEM306 (chemistry materials and methods) CHEM425 (advanced aspects of inorganic chemistry)
- E. Pahl taught 124.011, Foundation Studies Physics in the winter semester and is actually teaching the same paper in the summer school.
- P. Schwerdtfeger taught part of the Evolution paper, stage 2 biology (196.207) and first year Biochemistry 122.102 and 122.221.
- U. Zülicke taught a total of 100 Lectures and 26 Tutorials in physics papers (124.101, 124.102, 124.712) and in a nanoscience paper (236.201).
- A number of postdoctoral fellows (R. Tonner, D. Figgen, B. Assadollahzadeh, A. Borschevsky, and M. Wormit) and all PhD students contributed teaching in the chemistry labs, physics stage 1 teaching labs and astronomy labs.

Other activities:

Papers refereed:

- B. Assadollahzadeh refereed one paper for Nano Letters and one for J. Chem. Phys.
- P. Bowman refereed papers for Phys. Rev. Lett.
- K. Beloy refereed papers for Phys. Rev. A and Phys. Rev. Lett.
- J. Brand refereed papers for Phys. Rev. Lett., Phys. Rev. A, Physics Letters A, and Annalen der Physik.
- M. Lein refereed papers in Organometallics, J. Mol. Struct. THEOCHEM, Theor. Chem. Acc. and J. Comp. Chem.
- P. Schwerdtfeger refereed in total 80 papers from international journals including Angewandte Chem. Int. Ed., Chem. Commun., Chem. Phys. Chem., Chem. Phys. Lett., Chem. Europ. J., Inorg. Chem., J. Comput. Chem., J. Chem. Phys., J. Phys. Chem. A, J. Phys. Cond. Mat., Phys. Chem. Chem. Phys., Phys. Rev. A, Phys. Rev. B, Phys. Rev. Lett., Theoret. Chem. Acc. and many more.
- U. Zülicke refereed for Phys. Rev. Lett., Phys. Rev. B, EPL, Phys. Lett. A, Acta Physica Polonica.

PhD and MSc theses refereed:

- P. Bowman was Internal examiner for the MSc thesis of Julie Coxie and the PhD thesis of Christian Thierfelder.
- J. Brand: External examiner for PhD thesis of Bryan Wild, University of Otago.
- M. Lein: Internal examiner for the BSc (honours) thesis of Martin Heele.
- P. Schwerdtfeger: External examiner for the PhD thesis of P. Ingenhoven (Supervisor: U.

Zülicke), Massey University, PN, June 10; for G. McIntosh (Supervisor: Douglas Russell), Auckland University, June 12; and for Anna Gardens (Supervisor: Henrik Kjaergaard), Otago University, September 2.

- U. Zülicke: External examiner for the PhD thesis of Andrew Preston and Dmitri Schebarchev (both from VUW).

Conference Organisation:

- J. Brand organised a mini-symposium at the conference Nonlinear Wave 2010 at Tsinghua University, Beijing.
- P. Schwerdtfeger was the organizer of the Humboldt conference in Otago, January, 2010 with more than 150 participants from the New Zealand and Australian Humboldt Foundations together with highly acclaimed international guests. He was also on the organizing committee of 2 symposia at the *Pacificchem*, Hawaii, December 2010.
- R. Tonner was co-organizer of the Humboldt conference in Otago, January, 2010.

Chairs at Conferences:

- J. Brand chaired sessions at LPHYS'2010 in Iguazu (Brazil), Nonlinear Wave 2010 in Beijing, NIQuGas'10 in Ourense (Spain).
- T. Ernst chaired a session at the KOALA student conference 2010 in Dunedin.
- D. Figgen chaired a session at the Humboldt conference January 38-30 in Dunedin.
- A. Hermann chaired a session at the MacDiarmid Student and Postdoc Symposium in Wellington, November 2010. He also served as judge for student poster and talk competitions.
- P. Schwerdtfeger chaired sessions at the ICCMSE meeting in Greece and the Pacificchem Meeting in Hawaii. He also served as judge for student poster competitions and talks at the MM2010 meeting in Brisbane and the Pacificchem conference in Hawaii.

Editorial Boards / Professional Societies:

- P. Schwerdtfeger served on the editorial board for Journal of Computational Chemistry, Journal of Computational Methods in Sciences and Engineering, and Journal of Molecular Structure (Theochem). He also served as the President of the New Zealand Humboldt Association, for the election of Fellows to the Royal Society New Zealand, on the board of the Albany Leadership Forum, and on the board of the Asian-Pacific Association of Theoretical and Computational Chemists.

Community Outreach:

- P. Bowman delivered three talks to year 13 students at Orewa College and answered two questions for "Ask a Scientist", to be published in the Manawatu Standard.
- J. Brand gave a lecture on "Relativity" to year 13 students at Mahurangi College (4 August).
- D. Hallwood delivered a talk to year 13 students at Orewa College.
- E. Pahl hold Maths/Science extension classes to year 3 and 4 students at Albany Primary School.
- P. Schwerdtfeger gave a lecture "*From the Big Bang to the First Molecules in Life*", for school students, Sir Neil Waters Lecture Theatre, June 3; participated at the Emerging Researcher Network Function, Auckland, July 5. He was interviewed by Sunday Star Times for a newspaper article on the Humboldt Prize, which was published December 12. For press releases see:
<http://www.stuff.co.nz/sunday-star-times/features/4446393/Mysteries-of-our-time>
<http://www.royalsociety.org.nz/2010/12/06/fellow-awarded-humboldt-prize/>
- U. Zülicke was interviewed for and quoted in Rebecca Priestley's science column in the NZ Listener issue of 27 Nov 2010 "*Carbon's other face*".

PUBLISHED WORK

Papers published in refereed journals:

1. B. Assadollahzadeh, S. Schäfer, and P. Schwerdtfeger, "A Systematic Search for the Global Minimum Structures of Tin Clusters Sn_n ($n \leq 20$) and Corresponding Electronic Properties", *J. Comput. Chem.* **31**, 929-937 (2010).
2. J.Z. Bernád, M. Jääskeläinen, and U. Zülicke, "Effects of a quantum measurement on the electric conductivity: Application to graphene", *Phys. Rev. B* **81**, 073403-1-4 (2010). (*Selected for Virtual Journal of Nanoscale Science & Technology*).
3. J. Brand, T. J. Haigh, and U. Zülicke, "Sign of coupling in barrier-separated Bose-Einstein condensates and stability of double-ring systems", *Phys. Rev. A* **81**, 025602-1-4 (2010).
4. K. Beloy, "Lattice-induced non-adiabatic frequency shifts in optical lattice clocks", *Phys. Rev. A* **82**, 031402(R)-1-4 (2010).
5. K. Beloy, A. Borschevsky, P. Schwerdtfeger, and V. V. Flambaum, "Enhanced Sensitivity to the Time Variation of the Fine-Structure Constant and m_p/m_e in Diatomic Molecules: A Closer Examination of Silicon Monobromide", *Phys. Rev. A* **82**, 022106-1-7 (2010).
6. A. B. Chaplin, R. Tonner, and A. S. Weller, "Isolation of a low-coordinate rhodium phosphine complex formed by C-C bond activation of biphenylene", *Organomet.* **29**, 2710-2714 (2010).
7. J. C. H. Chen, O. Klochan, A.P. Micolich, A. R. Hamilton, T. P. Martin, L. H. Ho, U. Zülicke, D. Reuter, and A. D. Wieck, "Observation of orientation- and k-dependent Zeeman spin-splitting in hole quantum wires on (100)-oriented AlGaAs/GaAs heterostructures", *New J. Phys.* **12**, 033043-1-11 (2010).
8. J. J. Cooper, D. W. Hallwood, and J. A. Dunningham, "Entanglement-enhanced atomic gyroscope", *Phys. Rev. A* **81**, 043624 (2010).
9. B. Darquié, C. Stoeffler, S. Zrig, J. Crassous, P. Soulard, P. Asselin, T. R. Huet, L. Guy, R. Bast, T. Saue, P. Schwerdtfeger, A. Shelkownikov, C. Daussy, A. Amy-Klein, and C. Chardonnet, "Progresses toward a first observation of parity violation in chiral molecules by high-resolution laser spectroscopy", *Chirality* **22**, 870-884 (2010). (*review article for the Collet memorial issue*).
10. T. Ernst and J. Brand, "Resonant trapping in the transport of matter-wave solitons through a quantum well", *Phys. Rev. A* **81**, 033614-1-11 (2010).
11. T. Ernst, T. Paul, and P. Schlagheck, "Transport of ultracold Bose gases beyond the Gross-Pitaevskii description", *Phys. Rev. A* **81**, 013631-1-12 (2010).
12. D. Figgen, A. Koers, and P. Schwerdtfeger, "NWHCII - A small and compact chiral molecule with large parity violation effects in the vibrational spectrum." *Angew. Chem. Int. Ed.* **49**, 2941-2943 (2010). *Angew. Chem.* **122**, 3003-3005 (2010).

13. D. Figgen, T. Saue, and P. Schwerdtfeger, "Relativistic Four- and Two-Component Calculations of Parity Violation Effects in Chiral Tungsten Molecules of the Form NWXYZ (X, Y, Z = H, F, Cl, Br or I)." *J. Chem. Phys.* **132**, 234310-1-9 (2010).
14. A. Fotopoulos and M. Tsulaia, "On the Tensionless Limit of String theory, Off - Shell Higher Spin Interaction Vertices and BCFW Recursion Relations", *J. High Energy Phys.* **11**, 1-32 (2010).
15. A. Hermann, H. Gäggeler, and P. Schwerdtfeger, "Spin-orbit effects in structural and electronic properties for the solid-state of the group 14 elements from carbon to superheavy element 114", *Phys. Rev. B* **82**, 155116-1-8 (2010).
16. P. Ingenhoven, J.Z. Bernád, U. Zülicke, and R. Egger, "Features due to spin-orbit coupling in the optical conductivity of single-layer graphene", *Phys. Rev. B* **81**, 035421-1-6 (2010).
17. M. Jääskeläinen and U. Zülicke, "Anomalous spin-related quantum phase in mesoscopic hole rings", *Phys. Rev. B* **81**, 155326-1-6 (2010). (*Selected for Virtual Journal of Nanoscale Science & Technology*).
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