CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
NEW ZEALAND INSTITUTE FOR ADVANCED STUDY,
INSTITUTE OF NATURAL SCIENCES
and **INSTITUTE OF FUNDAMENTAL SCIENCES**
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To: Prof. Robert Anderson (PVC)

CTCP ANNUAL PERFORMANCE REPORT 2009

Activities and achievements: 2009 was again a successful year for our CTCP. One major new Marsden grant was awarded to Joachim Brand. Six other Marsden grants were still running in 2009. The total financial income from Marsden grants in 2009 was 1,375,000 NZ$, thus far exceeding all our running costs and salaries. Three new postdoctoral fellows joined our centre (Anastasia Borschevsky, Kyle Beloy and David Hallwood), and two PhD students (Brian Vest and Andreas Hermann) moved to short-term postdoctoral positions ending this year. A number of awards were received (the Royal Society's 2009 Hatherton Award for A. Hermann, the 2009 Massey University Early Career Research Medal for Matthias Lein, and the 2009 Massey University Individual Research Award and the Massey University College of Science Research Award for Peter Schwerdtfeger). Ralf Tonner received the prestigious Feodor-Lynen award of the German Alexander von Humboldt Foundation. A number of eminent long- and short-term scientists visited our research centre. The long-term visitors received funding from the international visitors fund of Massey University. On the publication side our centre produced 25 articles in internationally highly cited journals (10 papers in physics journals and 15 in chemistry journals). The many invitations to international conferences received by our academic staff clearly underline the reputation we have internationally.
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. The Helix-1 has now been officially decommissioned. This year we saw the failing of 4 nodes because of age, and further irreparable damage at 7 computer nodes due to a power cut. Aside from that, the Double-Helix computer ran without major down-time again for the whole year in 2009, which reflects the quality of the hardware provided by the Insite company. Both the Double-Helix and the BestGrid machines are used mainly by our research centre and are running at maximum capacity with 0% idle time. However, both machines are getting old and cannot satisfy our computational needs. Currently, computer jobs must be queued until many other jobs are completed, delaying important research output.
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.

Research Highlights: The research group headed by P. Schwerdtfeger discovered a chiral molecule with large parity violation effects. This is so far the best candidate for detecting parity violation for the first time. Moreover, investigations into the change of the fine-structure constants in space-time resulted in the prediction of some very promising diatomic molecules with detectable frequency drifts in the microwave spectrum (calculations are still

ongoing). For the recently predicted metallic phase transition of $CrCl_2$ under pressure the Max-Planck Institute in Stuttgart are preparing for experiments. Patrick Bowman and collaborators have scrutinised smearing techniques used to reduce the computational burden of frontline hadronic physics calculations. Such scrutiny became imperative as the results of such calculations have appeared in high-impact journals, such as *Science*. The group of Joachim Brand discovered a new way of creating particularly robust Schrödinger cat states of ultra-cold atoms rotating both left and right around a micrometer-sized ring trap. This discovery promises to have implications for future technologies of quantum-enhanced precision measurement and quantum information technology.

Future opportunities and directions: The ageing and slowly dying Double-Helix supercomputer at Albany has not been upgraded, and the chance of purchasing the anticipated Helix^3 (a Shared/Distributed Parallel Compute-Cluster) is close to zero. A major power cut in Albany destroyed seven of our units. I first pointed out some years ago that the computer room in Albany requires a power back-up generator, but nothing has been done to address this problem. In financial terms, the damage caused by the recent power cut is larger than the cost would have been for the purchase of a power generator. This clearly demonstrates that Massey University's policy of cost cutting and money saving can be self-defeating and lead to long-term damaging effects. Moreover, it is truly amazing that a research centre with such a large research income has no support for the purchase of a state-of-the-art computer like the anticipated Helix^3. Talks with the current VC indicate that no additional support will be forthcoming. We believe that the establishment of a major computational facility at Massey University is a university wide issue and of utmost importance. If Canterbury can do, why not Massey, the *defining* university? The current situation is not acceptable for our highly productive research centre. We are clearly an *internationally focused* (!) research centre, with strong national and international reputation, requiring support in terms of computer hardware by Massey University.

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 2009 by Joachim Brand jointly with Ulrich Zülicke, and we hope for more in 2010.

In summary, despite the set-backs on the computational side, it was again a great year for our research centre. 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 is reflected by the many invitations to present talks overseas, and by the many high-standing visitors who come to join our research centre for a certain time. We enjoyed constant moral and financial support from Nigel Long, Robert Anderson and Gaven Martin, and we really appreciate that. 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 much more.

Prof. Peter Schwerdtfeger
Date: December 17, 2009

Cc: Hon. Steve Maharey (VC), Prof. Nigel Long (DVC)
Prof. Gaven Martin (Director, INS and IAS), Prof. Peter Derrick (Director, 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: Kyle Beloy, Anastasia Borschevsky, Christian Thierfelder, David Hallwood, Ulrich 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)

Postdoctoral Fellows

Dr. Behnam Assadollahzadeh (Marsden fellow)
Dr. Anastasia Borschevsky (Marsden fellow, since November 2009)
Dr. Detlev Figgen (Marsden fellow)
Dr. Renyuan Liao
Dr. David Hallwood (Marsden Fellow)
Dr. Elke Pahl
Dr. Ralf Tonner (DAAD fellow and Alexander von Humboldt Feodor Lynen fellow)
Dr. Brian Vest (since May 2009)
Dr. Andreas Hermann (since July 2009)
Dr. Kyle Beloy (Marsden fellow, since October 2009)

Secretaries

Vesna Davidovic-Alexander (IAS)
Muharram Khoussainova (INS)

PhD Students

Susan Biering
Thomas Ernst
Andreas Hermann
Christian Thierfelder
Brian Vest

MSc Students

Julie Coxe
Jake Gulliksen

Exchange Students

Camilla Evangelisti (LMU Munich)
Anton Koers (Vrije Universiteit Amsterdam)
Philip Bron (Philipps Universität Marburg)
Claudia Loerbroks (Philipps Universität Marburg)
Urban Rohrmann (TU Darmstadt)

Visitors from other institutions:

Long Term:
Prof. Phil Bunker (NRC, Ottawa Canada)
Prof. Victor Flambaum (University of New South Wales)
Prof. Heinz Gäggeler (Bern University and PSI Villigen)
Prof. Qiang Gu (Beijing University of Science and Technology)
Prof. Dietmar Kolb (University of Kassel)
Prof. Michael Kuchiev (University of New South Wales)
Prof. Kirk Peterson (Washington State University)
Short Term:
Prof. Richard Bader (Mc Master, Ontario)
Prof. Rod Bartlett (University of Florida)
Prof. Peter Drummond (Swineburn University of Technology)
Prof. Gernot Frenking (Philipps University Marburg)
Sir Harold Kroto (Nobel Laureate, Florida State University)

Current Research Activities:

Cluster Simulations and Phase Transitions, Nanoscience
Density Functional and Ab-initio Theory
Transition Metal Catalysis and Theory of Chemical Bonding
Adsorption of organic molecules on semi-conductor surfaces
Surface enhanced Raman spectroscopy
Electroweak Electronic Structure Theory
Heterogeneous and Homogeneous Catalysis

High-Pressure Physics
Quantum Chromodynamics
Relativistic Quantum Chemistry
Nonlinear waves in Bose-Einstein Condensates
Quantum dynamics of ultra-cold few-atom systems
Strongly-correlated fermionic superfluids
One-dimensional quantum fluids
Solid State Physics
Superheavy Elements
Theoretical Inorganic and Organic Chemistry
Theory of functional nanostructures; Spintronics
Variation of Fundamental Constants in Space-Time

Grants Received/Continuing

- P. Bowman is in the second and final year of his Marsden Fast-Start for the project "*Bondage and Confinement: How Hadrons keep their Quarks*".
- J. Brand is in his second 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$670,000 in total (MAU0706). In addition he received another Marsden grant (09MAU048) on "*Icy tornadoes in the quantum world - Josephson junctions of Bose-Einstein condensates*" starting in 2010 (NZ$ $785,000).
- P. Schwerdtfeger is in his first year Marsden grant (together with V.V. Flambaum, Member of IAS) for the project "*The Variation of Fundamental Constants in Space-Time*" (2009-11), NZ$ 260,000 per annum for 3 years (08MAU070). He continues on 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, second year of funding (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, last year of funding (06MAU057). 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 has a continuing Marsden Grant (MAU0702). In addition, he is an AI on the newly funded Marsden application 09MAU048 (with J Brand).

Awards

- A. Hermann received the Royal Society's 2009 Hatherton Award for best student paper in the physical sciences (NZ$ 500), and Massey University's Dean's Award for Exceptional Thesis.
- M. Lein received the Massey University Research Medal (Early Career, NZ$ 10,000) 2009.
- P. Schwerdtfeger received both the Massey University Individual Research Award 2009 (NZ$ 20,000) and the Massey University College of Science Research Award 2009.
- R. Tonner started on a Feodor-Lynen fellowship of the German Alexander von Humboldt Foundation as post-doctoral (2 years of funding).

Ongoing MSc Theses

- J. Coxe: *Squeezing Atoms Using a Confinement Potential.* Supervisor: P. Schwerdtfeger
- J. Gulliksen: *Few-atom dynamics in a double-well potential*. Supervisor: J. Brand

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.

Finished PhD Theses

- 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. Thesis was handed in October 2009.

Lectures at Conferences / Meetings

- B. Assadollahzadeh gave an invited talk at the AMN-4 conference (University of Otago 8-12 February 2009) on "*From Clusters to the Solid State - Global Minimum Structures for Cesium Clusters and their Electronic Properties*".
- P. Bowman: "Centre vortices and the quark propagator in SU(2) and SU(3)", Invited talk at the 2nd Workshop on "*Nonperturbative Aspects of Field Theories"*, March 30 to April 3, 2009, Morelia, Mexico; "*Centre vortices and the quark propagator*", invited talk at Dynamics of Symmetry Breaking, Joint Theory Institute Workshop, April 13-17, 2009, Argonne National Laboratory, USA.
- J. Brand: Invited talks at international conferences: "*Classical and Quantum Dynamics of Josephson Vortices in tunnel-coupled Bose-Einstein condensates"* at Nonlinear Dynamics in Quantum Systems, Krasnoyarsk (Russia, 6/2009); "*Solitons and Macroscopic Quantum Tunneling of Bose-Einstein condensates in a Double-Ring Traps*" at Laser Physics (LPHYS'09), Barcelona (Spain, 7/2009); "*Rotational Schrodinger cat states with strongly interacting bosons*" at Quantum Chemistry and Quantum Computational Physics in the Theory of Ultra-cold Gases, Telluride (Colorado, 8/2009).
- D. Figgen: Contributed talk at the APCTCC-4 Conference in Malaysia on "*Parity violation: Why enantiomers differ in energy and how to prove it*" (12/2009).
- A. Hermann: Talk at AMN-4 conference on "*The optical spectrum of water*", Dunedin (February 8-12).
- M. Lein: Invited talk at the Meeting of the Asian Pacific Association of Theoretical and Computational Chemists (Malaysia, 12/2009) "*Homogeneous Gold Catalysis*".
- E .Pahl: Invited talk at AMN-4 conference in Dunedin (02/2009) titled *"Towards accurate melting temperatures from ab initio Monte Carlo simulations: from nano clusters to the bulk".*
- P. Schwerdtfeger: Invited/plenary talks on "*Science policy and funding in New Zealand*" at the Alumni Network Conference organized by the Foreign Office in Berlin, Germany (January 19-22); AMN-4 meeting in Dunedin on "*The Elusive Chromium Dihalide Structures - A Combined Computational and Gas Phase Electron Diffraction Study*" (February 8-12); International Conference on "Simulation and Dynamics for Nanoscale and Biological Systems in honour of Kimihiko Hirao's retirement, talk on "*From Small*

Clusters to the Liquid and Solid State – Simulation of Water and Rare Gases" (March 4-6); 13th ICQC International Conference on Quantum Chemistry, Helsinki, Finland, on "*Simulating mercury – from clusters to solids"* (June 22-27); Conference on Symmetries in Science, Bregenz, Austria, talk on "*Parity Nonconservation in Chiral Molecules*" (July 19-24); Gold Conference in Heidelberg on "*Periodic Trends and Relativistic Effects in the Group 11 Series of Elements*" (July 26-29); ACS Meeting Washington: Fluorine Chemistry Division on "*The Quest of Absolute Chirality*" (August 17), and Nuclear Division (Jeffrey Hay Symposium) on "*The Chemistry of Superheavy Elements*" (August 19); Molecular Modeling Meeting at Auckland University on "*Quantum Chemistry for Large Systems*" (September 11); ICCMSE Conference in Rhodos (Greece) on "*Detecting small effects in molecules: From Nuclear Hexadecapole Coupling to Parity Violation and the Change of Fundamental Constants in Space-Time*" (September 28 - October 4); Graz Humboldt Conference on Phenomenon Time – Dimensions and Structures in Culture and Science, on "*Albert Einstein's Concept of Relative Time*" (November 9-14).

- R. Tonner: Talk at the AMN-4 conference in Dunedin (02/2009) with the title: "*Adsorption of proline and glycine on the TiO_2(110) surface – a DFT study*".
- U. Zülicke: Invited talk *Spin-related quantum phases in mesoscopic hole rings* at the 2009 Gordon Godfrey Workshop on Spins and Strong Correlations, Sydney, Australia, 26 - 29 Oct 2009; Invited talk *Origin of larger-than-expected spin-interference effects in mesoscopic hole rings* at the International Symposium on Spin Manipulation in Solid State Systems, Würzburg, Germany, 8 - 9 Oct 2009; Invited talk *Rashba effect: Spin splitting of surface and interface states* at the 6th Annual Clusters and Nanoparticles Meeting, Lake Tekapo, New Zealand, 30 Nov – 1 Dec 2009.

Seminars and Talks

- P. Bowman gave a Seminar at the Nuclear Theory Center, Indiana University, USA on April 9, 2009.
- J. Brand: Bogoliubov Laboratory at the Joint Institute for Nuclear Research (Dubna, Russia, 6/2009); University of Amsterdam (8/2009).
- T. Ernst gave an invited talk at the Quantum Information group, University of Leeds, England on the 30th of June, 2009, "*Solitons in cold gases: Scattering on a well*".
- A. Hermann: Seminar at Friedrich Schiller University Jena (Germany); Seminar at University of Paderborn (Germany).
- M. Lein organized the CTCP Seminar series at Albany. He also presented a talk at Canterbury University on "*Scope and relevance of computational chemistry: from catalysis to weak electronic interactions*" (April 23).
- E. Pahl gave a seminar at University in Bratislava, Slovakia on *"Towards accurate melting temperatures from ab initio Monte Carlo simulations: from nano clusters to the bulk"* (7/2009).
- P. Schwerdtfeger gave invited talks at the Paul-Scherrer Institute in Villigen (Switzerland) on "*The Quest for Absolute Chirality*" (January 13), at the University of Stuttgart (Germany) on "*Relativistic Effects in the Chemistry of Gold*" (GdCH lecture, January 15); at the University of Freiburg (Germany) on "*The Chemistry and Physics of Superheavy Elements*" (June 29); Max-Planck Institute for Solid-State Research on "*The Nucleation of Chromium Dihalides*" (October 7); University of Cologne on "*The Quest for Absolute Chirality*" (November 19).
- U. Zülicke presented a contributed talk entitled *Spin-related geometric phase in mesoscopic hole rings* at the 4th International conference on Advanced Materials and Nanotechnology (AMN4), Dunedin, NZ, 8-12 Feb 2009.

Posters

- B. Assadollahzadeh presented a poster at the 13th ICQC International Conference on Quantum Chemistry, Helsinki, Finland, (22-27 June), on "*Global Minimum Structures of Small Nanoclusters and their Electronic Properties*".
- T. Ernst presented a poster at the Quantum Optics VII conference in Zakopane in Poland on the 8.6.-12.6, "*Scattering of a Soliton on a well*".
- E. Pahl presented a poster at the 13th ICQC International Conference on Quantum Chemistry, Helsinki, Finland, (22-27 June), on *"Towards accurate melting temperatures from ab initio Monte Carlo simulations: from nano clusters to the bulk".*
- R. Tonner presented a poster at the 13th ICQC International Conference on Quantum Chemistry, Helsinki, Finland, (22-27 June), on "*Adsorption of proline and glycine on the TiO_2(110) surface – a DFT study*".
- B. Vest presented a poster on "*The Nucleation of Chromium Dihalide Clusters*" at the 237th ACS national meeting in Salt Lake City, Utah.

Teaching

- P. Bowman taught parts of 124.101 and 124.102, stage 1 physics.
- J. Brand taught parts of 124.101 and 124.102, stage 1 physics.
- M.Lein taught parts of 124.101 (Lab course, chemistry) and 123.102 (Lectures, Physics).
- P.Schwerdtfeger taught part of the Evolution paper, stage 2 biology (196.207).
- U. Zülicke taught a total of 106 Lectures, 15 Tutorials, and 18 hours of Labs, spread over all levels of physics (124.101, 124.102, 124.226, 124.327, 124.712) and in nanoscience (236.201).
- A number of postdoctoral fellows (R. Tonner, D. Figgen, B. Assadollahzadeh and E. Pahl) and all PhD students contributed teaching in the chemistry and physics stage 1 teaching labs.

Other activities

Papers refereed:

- P. Bowman refereed papers for Physical Review Letters, Physical Review C, Physical Review D and Few-Body Systems.
- J. Brand refereed papers for Physical Review Letters, Physical Review A, New Journal of Physics, Journal of Physics B. Also served as external referee for staff promotion and departmental review (University of Otago).
- M. Lein refereed papers in Journal of Physical Chemistry, Theoretical Chemistry Accounts and Journal of Molecular Structure THEOCHEM.
- P. Schwerdtfeger refereed in total 69 papers from international journals including Angewandte Chem. Int. Ed. (9 papers alone this year), Chem. Commun., Chem. Phys. Chem. (6 papers), Chem. Phys. Lett., Europ. J. Inorg. Chem., Inorg. Chem., J. Comput. Chem., J. Chem. Phys., J. Phys. Chem. A (7 papers), J. Phys. Cond. Mat., Phys. Chem. Chem. Phys. (7 papers), Phys. Rev. A, Theoret. Chem. Acc., J. Mol. Struct. (Theochem.) and many more. He also reviewed grant applications from NSF (USA).
- R. Tonner refereed papers for Dyes and Pigments, J. Fluor. Chem., J. Organomet. Chem. and J. Phys. Chem. A.
- U. Zülicke refereed papers for Phys. Rev. Lett. (4), Phys. Rev. B (2), J. Appl. Phys. (1), Europhys. Lett. (1), Eur. J. Phys. B (2), Semicond. Sci. Technol. (1), Physica E (2).

PhD and MSc theses refereed:

- P. Bowman refereed one PhD thesis in Physics from the University of Adelaide and internal examiner for one Massey PhD thesis.
- J. Brand: External examiner for PhD thesis in Physics from the University of Queensland.
- M. Lein served as an outside assessor for the BSc (honours) thesis of Ms Jenna Burnie (University of Auckland).
- P. Schwerdtfeger: External examiner for the PhD thesis of Patryk Zaleski-Ejgierd (University of Helsinki).
- U. Zülicke: External examiner for PhD thesis in Physics of Andrew Preston (Victoria University of Wellington) and MSc thesis in Physics of Keryn Williams (Victoria University of Wellington).

Conference Organisation:

- J. Brand organised (with B.Blakie, M. Davis, and A. Bradley) *Cold Atom Theory* (Satellite to *Dodd-Walls Symposium*, Queenstown, 12/2008). Organiser (with L. Carr) of Minisymposium *Nonlinear Waves in Quantum Systems* at the conference *Nonlinear Waves 2010* in Beijing (6/2010).
- P. Schwerdtfeger was the organizer (together with M. Lein) of the *Relativistic Quantum Theory Symposium* as part of the WATOC International conference in September 2008; Organizer (together with P. Bunker) of the *High Resolution Spectroscopy Symposium* as part of the ICCMSE conference, Crete, October 2009; Co-organizer of the Humboldt meeting in Otago, January, 2010.
- R. Tonner is co-organizer of the Humboldt conference in Otago, January, 2010.

Chairs at Conferences:

- J. Brand chaired sessions at international conferences: Nonlinear Dynamics in Quantum Systems, Krasnoyarsk (Russia, 6/2009); Laser Physics (LPHYS'09), Barcelona (Spain, 7/2009).
- P. Schwerdtfeger chaired a whole day session at the ICCMSE conference, Crete, October 2009.
- U. Zülicke chaired a session on Modelling at the 4th International conference on Advanced Materials and Nanotechnology (AMN4), Dunedin, NZ, 8-12 Feb 2009.

Community Outreach:

- P. Bowman delivered a talk on particle physics to local school physics teachers and lead a discussion on solving scholarship exam problems at the Massey Physics Teacher meeting on the 25th of June, 2009.
- J. Brand delivered a talk on innovations in teaching Quantum Physics to physics school teachers from the Auckland region and lead a discussion on solving NCEA exam problems relating to that area.
- P. Schwerdtfeger was interviewed on Radio New Zealand National (Host: Bryan Crump, 22 Oct 2009); visited the New Zealand Embassador in Berlin to discuss science policies (January 19); was invited by the Foreign Office in Berlin to present an overview on science funding in New Zealand; hold meetings with representatives of the German Embassy in Wellington to discuss German - New Zealand science policies; Member of the Royal Society of New Zealand Fellowship Committee (Meeting Oct. 14 in Wellington).
- M. Lein and A. Hermann were interviewed for Radio New Zealand National ("Our changing world", to be broadcast in 2010).
- U. Zülicke presented a general talk *The universe in your pencil tip* at the Manawatu Physics Teachers' Meeting, Queen Elizabeth College, Palmerston North, 28 Aug 2009; and a general talk *Crooke's radiometer* as part of Science Week, Palmerston North Girls' High School, 19 May 2009.

PUBLISHED WORK

Papers published in refereed journals:

1. B. Assadollahzadeh, C. Thierfelder, P. Schwerdtfeger, "From clusters to the solid state: Global minimum structures for cesium clusters Cs_n (n=2-20,∞) and their electronic properties", *Phys. Rev. B* 78, 245423-1-11 (2008). (not listed in last years annual report)

2. B. Assadollahzadeh, P. Schwerdtfeger, "Global minimum structures and electronic properties for small gold clusters Au_n (n=2-20)", *J. Chem. Phys.* 131, 064306-1-11 (2009).

3. S. Biering, A. Hermann, J. Furthmüller, P. Schwerdtfeger, "The unusual solid state structure of mercury oxide: A first principle relativistic density functional study for the group 12 oxides ZnO, CdO and HgO", *J. Phys. Chem. A* 113, 12427-12432 (2009). (invited article, Pitzer Festschrift)

4. J. Brand, T. J. Haigh, U. Zülicke, "Rotational Fluxons of Bose-Einstein Condensates in Coplanar Double-Ring Traps", *Phys. Rev. A* 80, 011602-1-4 (R) (2009). [selected for Virtual Journal of Atomic Quantum Fluids]

5. A. Yu. Cherny, J.-S. Caux, J. Brand, "Decay of superfluid currents in the interacting one-dimensional Bose gas", *Phys. Rev. A* 80, 043604 (2009).

6. A. Yu. Cherny and J. Brand, "Dynamic and static density-density correlations in the one-dimensional Bose gas: Exact results and approximations", *Phys. Rev. A* 79, 043607 (2009).

7. D. Csontos, P. Brusheim, U. Zülicke, H. Q. Xu, "Spin-3/2 physics of semiconductor hole nanowires: Valence-band mixing and tunable interplay between bulk-material and orbital bound-state spin splittings", *Phys. Rev. B 79*, 155323-1-16 (2009). [selected for Virtual Journal of Nanoscale Science & Technology]

8. D. Figgen, P. Schwerdtfeger, "Structures, Inversion Barriers, and Parity Violation Effects in Chiral SeOXY Molecules (X, Y = H, F, Cl, Br or I)", *J. Chem. Phys.* 130, 054306-1-7 (2009). (invited article, Pitzer Festschrift)

9. D. Figgen, K. A. Peterson, M. Dolg, H. Stoll, "Energy-consistent pseudopotentials and correlation consistent basis sets for the 5d elements Hf–Pt" *J. Chem. Phys.* 130, 164108 (2009).

10. A. Hermann, P. Schwerdtfeger, "α-$CrCl_2$ under pressure: Prediction of a metallic phase transition", *J. Phys. Chem. A* 113, 12022-12027 (2009). (invited article, Thiel Festschrift)

11. P. Ingenhoven, R. Egger, U. Zülicke, "Spin transport and bipolaron density in organic polymers", *J. Phys.: Condens. Matter* 21, 415302-1-5 (2009).

12. B. Lange, R. Posner, R. K. Pohl, C. Thierfelder, G. Grundmeier, S. Blankenburg, W. G. Schmidt, "Water adsorption on hydrogenated Si(111) surfaces", *Surf. Sci.* 603, 60-64 (2009).

13. M. Lein, "Characterization of agostic interactions in theory and computation", *Coord. Chem. Rev.* 253, 625-634 (2009).

14. E. Pahl, F. Calvo, P. Schwerdtfeger, "The importance of accurate interaction potentials in the melting of argon nano-clusters", *Int. J. Quantum Chem.* 109, 1812-1819 (2009). (invited article, Hirao issue)

15. W. Petz, F. Öxler, B. Neumüller, R. Tonner, G. Frenking, "Carbodiphosphorane $C(PPh_3)_2$ as Single and Twofold Lewis Base with Boranes: Synthesis, Crystal Structures and Theoretical Studies of $H_3BC(PPh_3)_2$ and $[\{(\mu\text{-}H)H_4B_2\}C\{PPh_3\}_2]^+$", *Eur. J. Inorg. Chem.* 29, 4507-4517 (2009).

16. C. Thierfelder, P. Schwerdtfeger, "Effect of relativity and electron correlation in static dipole polarizabilities of ytterbium and nobelium", *Phys. Rev. A* 79, 032512-1-4 (2009).

17. C. Thierfelder, P. Schwerdtfeger, A. Koers, A. Borschevsky, B. Fricke, "Scalar relativistic and spin-orbit effects in closed-shell superheavy element monohydrides", *Phys. Rev. A* 80, 022501-1-10 (2009).

18. P. Schwerdtfeger, A. Hermann, "The equation of state for solid neon from quantum theory", *Phys. Rev. B.* 80, 064106-1-5 (2009).

19. P. Sebald, R. Oswald, P. Botschwina, H. Stoll, D. Figgen, "Accurate Potential Energy Surface and Calculated Spectroscopic Properties for CdH_2 Isotopomers", *J. Phys. Chem. A* 113, 11772-11782 (2009). (invited article, Thiel Festschrift)

20. B. Spohn, E. Goll, H. Stoll, D. Figgen, K. A. Peterson, "Energy-Consistent Pseudopotentials for the 5d Elements - Benchmark Calculations for Oxides, Nitrides, and Pt_2", *J. Phys. Chem. A* 113, 12478-12484 (2009). (invited article, Pitzer Festschrift)

21. R. Tonner, G. Frenking, "Divalent Carbon(0) Compounds.", *Pure Appl. Chem.* 81, 597-614 (2009).

22. R. Tonner, G. Frenking, "Tolman's electronic parameters for divalent carbon(0) compounds", *Organomet.* 28, 3901-3905 (2009).

23. B. Vest, P. Schwerdtfeger, M. Kolonits, M. Hargittai, "Chromium Difluoride: Probing the Limits of Structure Determination", *Chem. Phys. Lett.* 468, 143-147 (2009).

24. B. Vest, K. Klinkhammer, C. Thierfelder, M. Lein, P. Schwerdtfeger, "Kinetic and Thermodynamic Stability of Group 13 Trihydrides", *Inorg. Chem.* 48, 7953-7961 (2009).

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