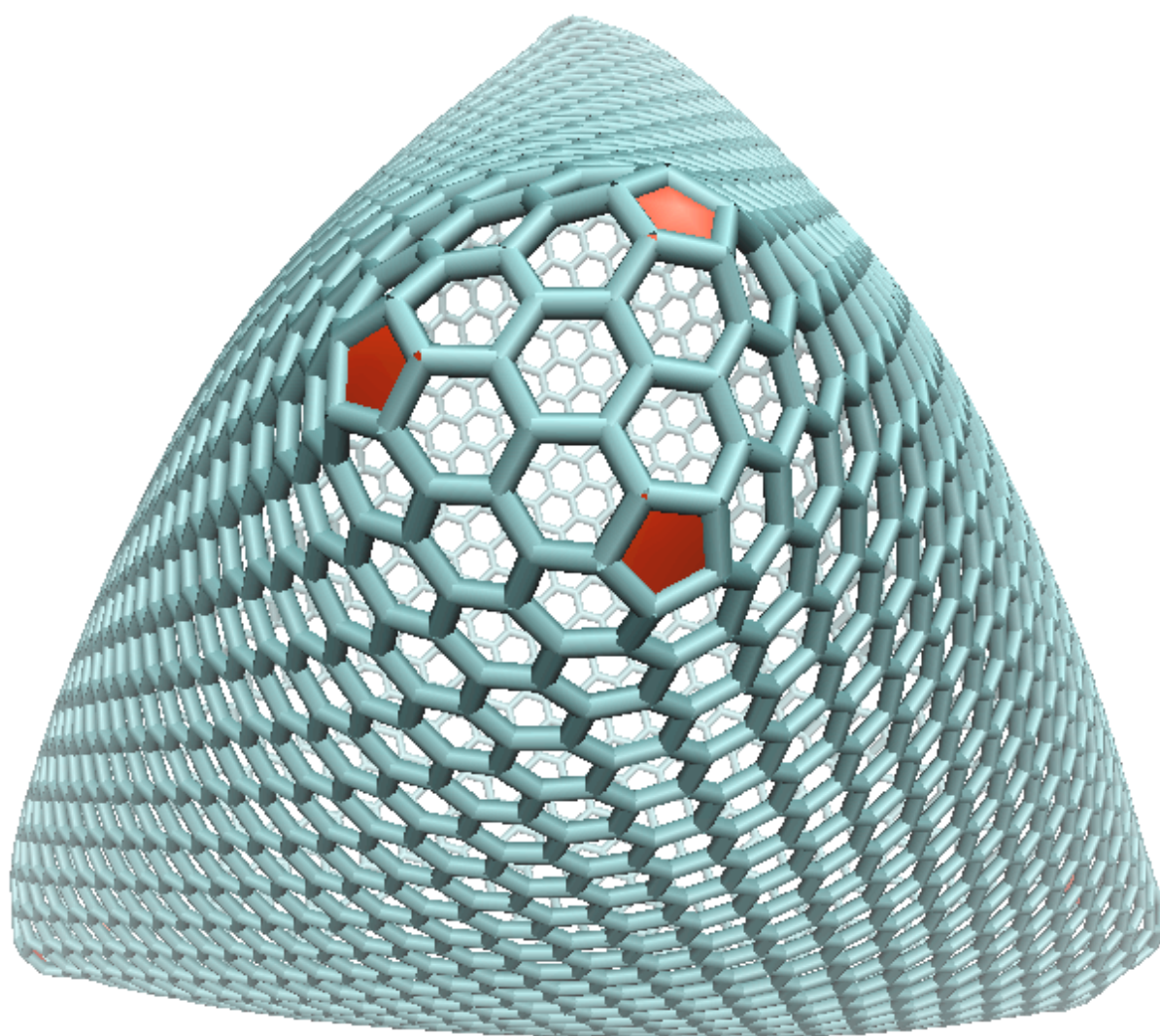


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**CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)**  
**NEW ZEALAND INSTITUTE FOR ADVANCED STUDY (NZIAS),**  
**INSTITUTE OF NATURAL AND MATHEMATICAL SCIENCES (INMS)**  
*Bldg. 40 and 44, Private Bag 102 904, North Shore MSC, Auckland, New Zealand*  
Ph: +64-9-4140800 ext. 435080, FAX: +64-9-443 9779  
Email: [p.a.schwerdtfeger@massey.ac.nz](mailto:p.a.schwerdtfeger@massey.ac.nz), Web: <http://ctcp.massey.ac.nz>

**2012 REPORT TO UNIVERSITY COMMERCIAL ACTIVITIES GROUP  
(CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS)**



The Second Halma Goldberg-Coxeter Transform of a  
 $C_{380}$  Fullerene Obtained with Program Fullerene

**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 are clearly met, as we are (to our knowledge) one of the most productive research centres here in New Zealand, with truly outstanding performances by each of our staff members. Our research centre has not been without a Marsden grant running since it was established. The many high-standing international visitors who joined our centre in 2012 are also an indication of our success.

**Research Output:** This year we published 40 articles in top journals and books amongst 7 permanent academic staff, again 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 year 1 level. All articles are published in highly acclaimed international journals of high impact factor such as *Physical Review Letters*. Amongst the outstanding achievements are the receipt of a Marsden fast-start grant by O. Fialko, the news feature on “The decay and collisions of dark solitons in superfluid Fermi gases” by Brand and co-workers (see <http://www.youtube.com/watch?v=kAQotOnD0mao>), and the election of P. Schwerdtfeger into the International Academy of Quantum Molecular Sciences (IAQMS), as well as the CMMSE prize for important contributions in the developments of Numerical Methods for Physics, Chemistry, Engineering and Economics (see <http://gsii.usal.es/cmmse>).

**The Future – Opportunities, Risks and Directions:** Our research centre is getting more diverse in research areas, and we need to discuss if the centre’s title (theoretical chemistry and physics) accurately describes the various activities. A discussion will take place in 2013. It was suggested to rename our centre to “Centre for Complex Systems”.

Another risk we can identify is the lack of top postgraduate students, as we do not offer a major in either chemistry or physics in Albany. Moreover, the physics side of research seems to dominate now, and chemistry in Albany needs some urgent future development plan. The lack of postgraduate students makes it very difficult to be competitive compared to other research groups worldwide.

Our main computational resource is the Double-Helix Supercomputer cluster, which consists of 35 dual processor HPC servers. The upgrade of the cluster to the Bright Cluster Manager software tool (see <http://www.brightcomputing.com/Bright-Cluster-Manager.php>) running on top of Scientific Linux 6 has been completed. Together with the relocation of the head-node, this has improved the run-time stability of the cluster immensely. Now that the most important quantum chemistry and physics program packages have been installed and optimised, a large number of MU users are making heavy usage of the system with basically little idle time.

By demonstrating the demand for computational resources within the research centre and the two institutes IAS and INMS, we have secured a grant of 90,000 \$ from the science faculty to invest in more hardware. This funding will allow us to increase in the capacity of the cluster by about 50%. This extra investment will be crucial as the new Molecular Dynamics (Jane Allison) and Complex Systems groups (Sergej Flach) ramp-up their usage.

The CTCP desktop system's storage array has been upgraded and the system is running well. The individual desktop operating system will have to be upgraded in the upcoming year, which will require a considerable amount of staff time.

We are still working on integrating our systems with the Best-Grid cluster and other systems within the College of Science. We are optimistic that this will reduce the administration overhead in the long-term, but our progress is currently limited by lack of available time for system administration. This should be rectified with the arrival of the new research officer.

**Work in progress:** There are too many research projects in progress to list all of them (see attachment for more details). Funding in 2013 is anticipated mainly through Marsden Grants. A 90,000\$ grant by Massey University College of Science will be used to upgrade our Double-Helix Supercomputer cluster.

**Staffing:** 2012 saw the addition of two new academic staff member, Prof. Sergej Flach (Mathematical Physics) and Dr. Jane Allison (Biomolecular Simulation). Both groups will use the CTCP Double-Helix Super-computer cluster. Several postdoctoral fellows left (Dr. Kyle Beloy, Dr. Susan Biering, Dr. Anastasia Borschevsky, Dr. Andreas Hauser and Dr. Michael Wormit). Hence the theoretical chemistry section has the lowest number of researchers since it was established in 2003. The good news is that Dr. Florian Senn joined our research centre beginning of 2012. He is financed by the Swiss Science Foundation.

**Financial:** See attachment

**Acknowledgment:** The Director likes to thank all CTCP members for their outstanding performance and their hard work in 2012, and wishes everybody a successful 2013. We enjoyed constant moral and financial support from Prof. Robert Anderson. Finally, my very special thanks goes to our Institute's secretary, Mrs Vesna Davidovic-Alexander (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).



Dist. Prof. Peter Schwerdtfeger  
Director of CTCP, DHOI NZIAS

**Date:** February 7, 2013

Cc: Hon. Steve Maharey (VC), Prof. Gaven Martin (Director, INS and IAS), Prof. Brigid Heywood (Assistant VC Research), Prof. Robert Anderson (Pro-VC Science).

## Appendix



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

*Daniel Götz, Elke Pahl, Urban Rohrmann, Likas Wirz, Jane Allison, Alberto Cetoli, Mark Hoffmann (Visitor), Florian Senn, Peter Schwerdtfeger, Patrick Bowman, Joachim Brand, Sergej Flach, Vesna Davidovic-Alexander, Carlo Danieli, James Avery, Andrew Punnet, Jonas Wiebke, Kristian Rayanov, Oleksandr Fialko, Mustafa Hasanbulli. Missing in this picture: Thomas Ernst, Anastasia Borschevsky, Andreas Hauser, Michael Wormit, Mustafa Hasanbulli, Susan Biering, Ulrich Zülicke (Victoria University of Wellington), Gabriele Jaritz, and Tilo Söhnel.*

### **Personnel:**

Prof. Peter Schwerdtfeger (Chemistry, Director of CTCP)

Prof. Joachim Brand (Physics, Deputy Director of CTCP)

Prof. Sergej Flach (Physics)

Dr. James Avery (Research Officer, until July 2012)

Dr. Patrick Bowman (Senior Lecturer, Physics)

Dr. Elke Pahl (Lecturer, Physics)

Dr. Jane Allison (Lecturer, Biological Sciences)

### **Honorary CTCP Members:**

Dr. Matthias Lein

Dr. Tilo Söhnel

Prof. Uli Zülicke

### **Secretaries:**

Vesna Davidovic-Alexander (IAS)

Muharram Khoussainova (INS)

### **PhD Students:**

Mustafa Hasanbuli (Supervisor: P. Schwerdtfeger)  
Lukas Wirz (Supervisors: P. Schwerdtfeger and J. Allison)  
Andrew Punnett (Supervisor: P. Bowman)

### **MSc Students:**

Gabriele Jaritz (Supervisor: J. Brand)

### **Exchange Students:**

Sebastian Gohr, FU Berlin, MSc Thesis: “CO<sub>2</sub> under Pressure – A Computational Study”  
(Supervisors: P. Schwerdtfeger, T. Söhnel and B. Paulus)  
Daniel Götz, Darmstadt, PhD studies on gold and lead clusters

### **Research Assistant:**

Sophie Shamailov (Supervisor: J. Brand)

### **Postdoctoral Fellows:**

Dr. Kyle Belay (Marsden fellow, until January 2012)  
Dr. Susan Biering (Honorary Research Fellow)  
Dr. Anastasia Borschevsky (Marsden fellow, until August 2012)  
Dr. Alberto Cetoli (Wenner-Gren Postdoctoral Fellow)  
Dr. Oleksandr Fialko (Marsden fellow)  
Dr. Andreas Hauser (Postdoctoral fellow until March 2012)  
Dr. Florian Senn (Swiss Science Foundation)  
Dr. Michael Wormit (Alexander von Humboldt Feodor Lynen fellow, until June 2012)  
Dr. Jonas Wiebke (DAAD fellow)

### **Visitors from other institutions:**

#### *Long Term:*

Prof. Victor Flambaum (University of New South Wales)  
Dr. Renyuan Liao (Chinese Academy of Sciences)  
Prof. Per Jensen (University Wuppertal, Germany)  
Shih-Wei Su (National Tsinghua University, Taiwan)

#### *Short Term:*

Prof. Peter Drummond (Swinburne University of Technology, Australia)  
Prof. Heinz Gaeggeler (PSI, Bern University, Switzerland)  
Prof. Rhett Kempe (University of Bayreuth, Germany)  
Dr. Maxim Pospelov (Perimeter Institute for Theoretical Physics, Ontario, Canada)  
Dr. Dmitri Scherbachov (IRL, Wellington)  
Dr. Shi Wei Si (National Changhua University of Education, Taiwan)  
Prof. Klaus Ziegler (University of Augsburg, Germany)

### **Current Research Activities:**

Cluster Simulations and Phase Transitions, Nanoscience  
Development of new methods for electronic structure calculations  
Frequency shifts in atomic clocks  
Electroweak Electronic Structure Theory  
Generalized Sturmian methods for many-body problems  
Graph theoretical and topological properties of fullerenes  
Heterogeneous and Homogeneous Catalysis

High-Pressure Physics  
 Macroscopic quantum superpositions  
 Nonlinear waves in Bose-Einstein Condensates  
 Nonlinear classical and quantum waves in disordered potentials  
 Non-perturbative QED  
 Password encryption with nonlinear waves at phase transitions  
 Polariton condensate network dynamics  
 Non-equilibrium phase transitions  
 One-dimensional quantum fluids  
 Quantum Chromodynamics  
 Quantum dynamics of ultra-cold few-atom systems  
 Quantum enhanced precision measurement  
 Quantum ratchets with ultracold atomic gases  
 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  
 Topological and Graph Theoretical Aspects of Fullerenes  
 Transition Metal Catalysis and Theory of Chemical Bonding  
 Parity violation in molecules  
 Variation of Fundamental Constants in Space-Time  
 Biomolecular simulation

### Grants Received/Continuing:

- J. Allison, S. Flach and P. Schwerdtfeger: Massey University Capital Expenditure Grant for upgrading the double-helix compute cluster
- J. Brand: Ongoing Marsden grant on “Icy tornados in the quantum world: Josephson Junctions of Bose-Einstein condensates” (since 2010).
- Oleksander Fialko: Marsden FastStart on “Understanding quantum thermodynamics with the smallest heat engine” (starting 2013).

### Honours and Awards:

- A. Borschevsky received the Helmholtz-Institute Mainz Visiting Researcher Grant (Institute Mainz Internationales Gastwissenschaftlerprogramm). The purpose of the grant was to allow her to spend a month as a visiting scientist at the GSI Helmholtz Centre in Darmstadt, Germany, and to attend the ENSAR-ECOS Workshop on Future of Superheavy



**RECOGNISING EXCELLENCE IN RESEARCH.**

Recently the Marsden Fund awarded more than \$5.5 million to six of Massey University's research projects and two of our most outstanding researchers in the early stages of their careers.

We would like to congratulate:

- MARY MORGAN-RICHARDS, Institute of Natural Resources
- PHIL BATTLEY, Institute of Natural Resources
- PAUL PLIEGER, Institute of Fundamental Sciences
- GAVEN MARTIN, New Zealand Institute for Advanced Study
- REGINA SCHEVENS AND GLENN BANKS, School of People, Environment and Planning
- HELEN MOEWAKA BARNES, Te Pūnui Whāiriaki
- OLEKSANDR FIALKO, New Zealand Institute for Advanced Study
- IMRAN MUHAMMAD, School of People, Environment and Planning

All Massey University our students and staff truly are the engine driving change in the new New Zealand, and globally.

MASSEY.AC.NZ

THE ENGINE OF THE NEW ZEALAND

- Element Strategy (FUSHE2012), in Weilrod, and the Physics Prospects at FLAIR - The Facility for Low-Energy Antiproton and Ion Research Workshop, in Darmstadt, Germany.
- Dr. Alberto Cetoli has been awarded a prestigious post-doctoral scholarship from the Wenner-Gren foundation. The Wenner Gren foundation will fully support Alberto for one year (extendible for another year) to work on the project "Dark solitons in superfluid Fermi gases".
  - P. Schwerdtfeger became Distinguished Professor at Massey University, and has been elected into the International Academy of Quantum Molecular Sciences (IAQMS). The Academy is composed of persons chosen amongst the scientists of all countries who have distinguished themselves by the value of their scientific work, their role as pioneer or leader of a school and have most contributed to the advancement of quantum molecular sciences. The Academy currently has 107 members and Its headquarter is in Menton (France). Peter is the first New Zealand scientist to receive this honour. He also received the CMMSE prize given to computational researchers for important contributions in the developments of Numerical Methods for Physics, Chemistry, Engineering and Economics (<http://gsii.usal.es/cmmse>).
  - L. Wirz received the inaugural Sir Neil Waters Scholarship.

### Publicity:

- Prof. J. Brand's news feature on "The decay and collisions of dark solitons in superfluid Fermi gases" by Brand and co-workers:  
(see <http://www.youtube.com/watch?v=kAQtOnD0mao>)
- Dr. Andreas Hauser and Prof. Peter Schwerdtfeger's work on graphene nanopores has been highlighted in an article on the Royal Society of Chemistry News Magazine "Chemistry World" (<http://www.rsc.org/chemistryworld/2012/05/gas-separation-graphene-nanopores>). The group has performed ground-breaking work on the use of porous graphene membranes to separate Helium-3 and Helium-4 isotopes. This fundamentally quantum process is very exciting and has many potential applications in fields ranging from environmental protection to nuclear fusion.

### Ongoing PhD Theses:

- M. Hasanbulli (second year): *Atoms in Spherical Confinements*. Supervisors: P. Schwerdtfeger and B. Pavlov
- A. Punnett (fourth year): *How Hadrons keep their Quarks*. Supervisor: P. Bowman.
- Lukas Wirz (first year): Computer Modelling of Fullerenes / Biasing molecular modelling with experimental RDCs. Supervisors: P. Schwerdtfeger and J. Allison

### Finished MSc Theses:

- Gabriele Jaritz: *Icy tornadoes in the quantum world – Josephson junctions in Bose-Einstein condensates*. Supervisors: J.Brand and U. Zuelicke (December 2012 / January 2013)

### Lectures at Conferences / Meetings:

- J. Allison was an invited speaker at i) the Molecular Modelling - 2012: Discovery through Biomolecular Simulation meeting of the Association of Molecular Modellers of Australasia, Queenstown, NZ (August 2012), where she gave a talk entitled "*Enhancing biomolecular simulations with experimental data (and vice versa)*"; and ii) the Biomolecular Interaction Centre 2<sup>nd</sup> Birthday Symposium, Christchurch, NZ (April 2012), where she gave a talk entitled "*What biomolecular modelling can (and cannot) do for you*".

- J. Avery was an invited speaker at the conference MEST 2012: *Molecular Electronic Structure at Troy*, September 9<sup>th</sup> to 13<sup>th</sup> in Çanakkale, Turkey. He gave a lecture titled “*Efficient Multi-Center Electron Repulsion Integrals for Exponential Type Orbitals: Two New Methods*”.
- A. Borschevsky gave talks at the Heavy Ion Accelerator Symposium (HIAS2012), in Canberra, Australia (*Chemical Properties of the Superheavy Elements: Theory and Experiment*) and at the 48<sup>th</sup> Symposium on theoretical Chemistry (STC2012), in Karlsruhe, Germany (*Benchmark Calculations of Atomic Properties of Element 120*). She also participated in the ENSAR-ECOS Workshop on Future of Superheavy Element Strategy (FUSHE2012), in Weilrod, Germany, and in the Physics Prospects at FLAIR - The Facility for Low-Energy Antiproton and Ion Research Workshop, in Darmstadt, Germany.
- J. Brand gave invited talks at the following conferences: “Winter Colloquium on the Physics of Quantum Electronics” in Snowbird, Utah, January 2-6 (2012); 20<sup>th</sup> International Laser Physics Workshop in Calgary, Canada, July 23-27 (2012); University of Queensland Workshop on Quantum Gases, November 18 – December 2 (2012).
- S. Flach: gave i) an invited talk at the 2012 conference Disordered Quantum Systems in Paris (France, June) on “*Nonlinear waves in disordered systems*”; ii) an invited talk at the 2<sup>nd</sup> Conference on Localized Excitations in Nonlinear Complex Systems 2012 in Sevilla (Spain, July) on “*Correlated metallic two-particle bound states in quasiperiodic chains*”; iii) an invited talk on at the 2012 Quantum Days Bilbao in Bilbao (Spain, July) on “*Nonlinear waves in complex systems*”; iv) three tutorial lectures at the 2012 Advanced Workshop on Energy Transport in Low-Dimensional Systems in Trieste (Italy, October) on “*Nonlinear waves in low-dimensional systems: problems, essentials, perspectives*”; v) a plenary lecture at the 2012 Dynamics Days South America in Cartagena (Colombia, November) on “*Nonlinear waves in complex systems: problems, essentials, perspectives*”;
- E. Pahl took part in the Conference on Mathematical Methods in Science and Engineering (CMMSE) in Murcia, Spain and gave an invited talk on “Simulation of Mercury Melting: A Hard Nut to Crack”. She also gave a talk about “Quantum Physics” at conference for gifted teenagers, NZAGC in Auckland.
- P. Schwerdtfeger participated at the 2012 Workshop on Theoretical Chemistry in Kathmandu (Nepal). There he gave a plenary lecture on “*High Pressure Simulations – Squeezing the Hell out of Atoms*” (April 28). He also participated at the 12<sup>th</sup> International Conference on Mathematical Methods in Science and Engineering (CMMSE) 2012 in Murcia (Spain) and gave a plenary lecture as well on “*High Pressure Simulations – Squeezing the Hell out of Atoms*”. At the TACC (Theory and Applications of Computational Chemistry) 2012 conference in Pavia (Italy), Peter gave an invited keynote lecture on “*The Relativistic Pseudopotential Approximation*” (September 5). He also gave an invited lecture at the REHE (Relativistic effects in heavy elements) 2012 conference on “*The variation of fundamental constants in space-time*” (September 12).
- U. Zülicke was an invited speaker at the March Meeting of the American Physical Society, Boston, USA, 27 February – 2 March 2012. His talk entitled “*Quantum-confined holes: More spin for your buck!*” was part of a Focus Session on Spins in Semiconductors. Uli also spoke at the UQ Quantum Gas Workshop 2012, Brisbane, Australia, 19 – 30 November 2012 about “*Low-dimensional spin-orbit-coupled BECs: Inspirations from semiconductor spintronics*”.



## Seminars and Talks:

- J. Allison gave seminars at i) Massey University, Palmerston North, NZ (May 2012) and ii) Victoria University, Wellington, NZ (July 2012) entitled “*Shake, rattle and roll: using simulations to explore how proteins move*”; iii) University of Auckland, NZ (November 2012), iv) University of Natural Resources and Life Sciences, Vienna, Austria, and v) King’s College London, UK, entitled “*And yet it moves: combining experiment and simulation to describe how proteins really (mis)behave*”; and vi) ETH Zürich, Switzerland entitled “*Modelling an evolutionary arms race*”.
- J. Avery gave a seminar on November 7<sup>th</sup> at Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China. The seminar was titled “*A Brief Overview of Experimental Mathematics*”.
- S. Biering was invited to give a talk titled “A comparative DFT study of the solid group 12 chalcogenides: Trends and relativistic effects” at the Department of Physical and Theoretical Chemistry, Freie Universität Berlin, Berlin, Germany (June 2012).
- A. Borschevsky gave a seminar at the Centre for Theoretical Chemistry and Physics, Massey University, Auckland, New Zealand (16/03/2012). Topic: “*Benchmark calculations of atomic properties of the superheavy elements*”.
- O. Fialko gave a talk at the Swinburne University of Technology, Melbourne, Australia. Group of Prof. Peter Drummond.
- S. Flach: gave i) a colloquium at the Asia-Pacific Centre for Theoretical Physics in Pohang (South Korea, May 2012) on “*Nonlinear waves in complex systems: problems, essentials, perspectives*”; ii) two colloquia at the University of Chile at Santiago de Chile and the Catholic University at Santiago de Chile in November 2012 on “*Nonlinear waves in complex systems: problems, essentials, perspectives*”; iii) a lecture course of seven lectures at the Tbilissi State University (Georgia) in December 2012 on “*Nonlinear classical and quantum waves in complex systems*”.
- E. Pahl gave a talk about “Melting of nanoclusters” at the University of Heidelberg, Germany in July 2012.
- P. Schwerdtfeger was invited as an international guest speaker at the University of Tennessee for the annual fund raising event at the University of Tennessee, March 5. He gave a lecture on “*The variation of fundamental constants in space-time*”. The day after he gave a talk at Oak Ridge National Laboratory on “*The chemistry and physics of superheavy elements*”. April 10 he gave a talk on “*Of Spheres, Fullerenes, Hyperfullerenes and Graphene*” at the University in Bochum, and April 11 on “*The Relativistic Pseudopotential Approximation*”. On April 25 Peter gave an invited lecture at Marburg University, organized by the German Chemical Society (GDCh), on “*Left or right in nature? The origin of biomolecular homochirality*”. He visited the Facultad de Ciencias, Universidad Autonoma de Madrid, and gave a talk on “*Topological and graph theoretical aspects of fullerenes*” (July 11). The following day Peter visited the CSIC National Laboratory in Madrid, an organization similar to our CoREs in New Zealand. There he gave a talk on “*Toward the detection of parity violation in chiral molecules*”. On August 22 he visited Freiburg University, to give a talk on “*High Pressure Simulations – Squeezing the Hell out of Atoms*”.
- U. Zülicke gave invited seminar presentations with the title “*Quantum-confined holes: More spin for your buck!*” at the Department of Physics, University of Texas, Austin, Texas, USA, on 21 February 2012, and the Department of Physics, University of Basel, Switzerland, on 4 April 2012.

## Posters:

- O. Fialko gave a poster presentation at the "Frontiers of Cold Atoms and Related Topics" conference, May 14-17, 2012, Hong Kong.
- E. Pahl gave a poster contribution at the ESPA 2012 in Barcelona, Spain titled "Toward the Melting of Mercury: A Challenge to Computational Chemistry".

## Teaching:

- J. Allison taught into 122.102 Biochemistry of Cells, 123.172 Chemistry for Biological Systems, 246.201 Science and Sustainability and 122.704 Molecular Cell Biology.
- S. Biering demonstrated in the stage 1 physics labs.
- P. Bowman was paper coordinator for 124.101 and 124.171 and taught parts of 124.102/172, stage 1 physics/engineering, and was paper coordinator for 124.129 Astronomy. He also taught into the new B.Nat.Sci paper 246.102.
- J. Brand taught parts of 124.101 and 124.102, stage 1 physics and part of 124.129 Astronomy. J. Brand also gave a lecture course at the Victorian Summer School in Ultracold Physics (Melbourne, June/July 2012) on the physics of ultracold Bose gases in one-dimensional and ring traps.
- E. Pahl taught parts of 124.111, stage 1 physics and was paper coordinator of this paper. She also taught into the "Science and Sustainability" paper, 246.101.

## Other activities:

### *Papers refereed:*

- J. Allison refereed papers for the Journal of Chemical Theory and Computation, ChemPhysChem, and Computational and Mathematical Methods in Medicine, and reviewed grant applications for EPSRC (UK).
- P. Bowman refereed papers for Physical Review Letters and Physical Review D.
- J. Brand refereed papers for Physical Review Letters, Physical Review A, New Journal of Physics, Europhysics Letters, European Journal of Physics D, Frontiers of Physics, Fortschritte der Physics – Progress of physics, and Physica D.
- P. Schwerdtfeger refereed in total 57 papers (rejecting about 50% of the invitations) from international journals including Angewandte Chem. Int. Ed., Chem. Phys. Chem., Chem. Phys. Lett., Chem. Europ. J., 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.

### *PhD and MSc theses refereed:*

- P. Bowman refereed the MSc thesis of Gabriele Jaritz (Massey University, Supervisor Joachim Brand) on "Icy tornadoes in the quantum world: Josephson junctions of Bose-Einstein condensates".
- S. Flach refereed the 2012 PhD thesis of Taegeun Song (Chungnam University, Supervisor Kang-Hun Ahn) on "Characteristics and Mechanisms in a Quantum Point Contact and an Artificial Hair Cell".
- P. Schwerdtfeger refereed one PhD thesis in 2012: Philip McGill (Auckland University, Supervisors: Hicham Idriss and Tilo Söhnel) on "Theoretical Studies of Model Molecule Adsorption to the Surfaces of Titania and Ruthenium".

#### *Conference Organisation:*

- J. Brand co-organized the Victorian Summer School in Ultracold Physics in Melbourne, June/July 2012.
- P. Schwerdtfeger organized a symposium on “*From small clusters to the solid phase*” at the 12<sup>th</sup> International Conference on Mathematical Methods in Science and Engineering (CMMSE) 2012 in Murcia (Spain), July 2-6.

#### *Conference Participation:*

- O. Fialko participated at the "Quantum Gas Workshop", 18 - 29th November 2012, Brisbane, Australia.

#### *Chairs at Conferences:*

- J. Brand chaired a session at the 20<sup>th</sup> International Laser Physics Workshop in Calgary, Canada, July 23-27 (2012)
- P. Schwerdtfeger chaired a session at the 12<sup>th</sup> International Conference on Mathematical Methods in Science and Engineering (CMMSE) 2012 in Murcia (Spain), July 2-6.

#### *Boards / 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 Wiley Interdisciplinary Reviews: Computational Molecular Science. He also served as the President of the New Zealand Humboldt Association, and served on the board of the Asian-Pacific Association of Theoretical and Computational Chemists. Further he served as a member of the Academic Leadership team and of the INMS Exec Board at MU.

#### *Community Outreach:*

- S. Biering took part in the “Rotary National Science & Technology Forum”, mentoring and demonstrating for high achieving year 12 students that are interested in science. (Jan. 2012) - (I also have been a demonstrator for the “Long Night of Science”, a community outreach programme at the Freie Universität Berlin, Berlin, Germany (June 2012).
- P. Bowman gave talks about Electromagnetism to students at Glenfield college and Mahurangi College.
- E. Pahl gave a talk about Quantum Physics at a conference for gifted teenagers in Auckland together with J. Brand.

#### *Visits:*

- S. Biering spent two month at the Freie Universitaet Berlin, Berlin, Germany (April-June 2012), where she collaborated with Beate Paulus (Department of Physical and Theoretical Chemistry) on the absorption of Pyridine on Au(100) Surfaces.
- A. Borschevsky spent a month as a visiting scientist at the GSI in Darmstadt, Germany (May 2012).
- P. Schwerdtfeger participated in a superheavy element (the FUSHE group) meeting at the GSI in Darmstadt to collaborate on joint superheavy element research (August 31). He also visited the University of Castilla - La Mancha in Spain just north of Granada (Toledo and Ciudad Real), a multi-campus university just like ours with four campus sites. Particularly interesting was the environmental chemistry program, which the university runs with great success.

## PUBLISHED WORK

Articles published in 2012 refereed journals (members of CTCP are in bold letters):

1. J.S. Avery, **J.E. Avery**, “Coulomb Sturmians as a basis for molecular calculations”, *Molecular Physics* 110, 1593-1608, Taylor and Francis 2012. doi: 10.1080/00268976.2012.658876
2. **J. R. Allison**, “Assessing and refining molecular dynamics simulations of proteins with nuclear magnetic resonance data”, *Biophys. Rev.* 4, 189-203 (2012).
3. **S. Biering, P. Schwerdtfeger**, “A comparative density functional study of the low pressure phases of solid ZnX, CdX and HgX. Trends and relativistic effects”, *J. Chem. Phys.* 136, 034504-1-15 (2012).
4. **S. Biering, P. Schwerdtfeger**, “A comparative density functional study of the high-pressure phases of solid ZnX, CdX and HgX (X=O, S, Se and Te): Trends and relativistic effects”, *J. Chem. Phys.* 137, 034705-1-17 (2012).
5. **A. Borschevsky, M. Ilias, V. A. Dzuba, K. Beloy, V. V. Flambaum, P. Schwerdtfeger**, “The  $P$ -odd interaction constant  $W_A$  from relativistic *ab initio* calculations of diatomic molecules”, *Phys. Rev. A* 85, 052501-1-7 (2012).
6. **A. Borschevsky, M. Ilias, V. A. Dzuba, K. Beloy, V. V. Flambaum, P. Schwerdtfeger**, “Nuclear-spin dependent parity violation in diatomic molecular ions”, *Phys. Rev. A* 86, 050501-1-4(R) (2012).
7. **A. Borschevsky, T. Zelovich, E. Eliav, and U. Kaldor** “Precision of calculated static polarizabilities: Ga, In and Tl atoms”, *Chem. Phys.* 395, 104-107 (2012).
8. F. Calvo, **E. Pahl, P. Schwerdtfeger**, F. Spiegelman, “Diatomics-in-molecules modeling of many-body effects on the structure and thermodynamics of mercury clusters”, *J. Chem. Theory Comput.* 8, 639-648 (2012).
9. A. Cetoli, C. J. Pethick, “Interaction of gravitational waves with matter”, *Phys. Rev. D* 85, 064036-1-9 (2012)
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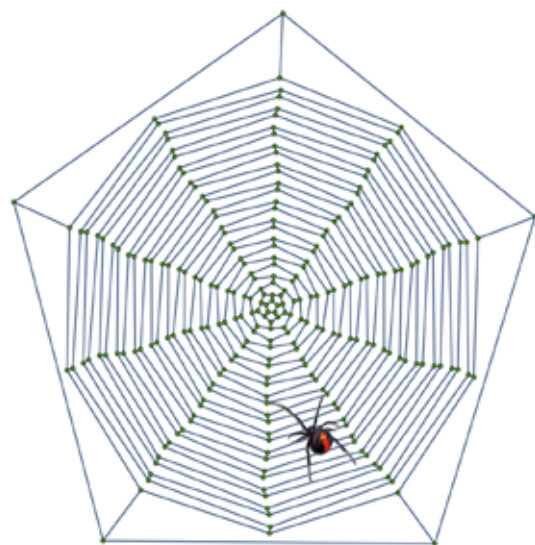
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### Software developments:

- P. Schwerdtfeger, L. Wirz and J. Avery: Software package *Fullerene Version 4.4* available under open source and can be found online at Massey University web-site <http://ctcp.massey.ac.nz/index.php?group=&page=fullerenes&menu=fullerenes>



*Program Fullerene is a Fortran code, which performs a topological and graph theoretical analysis of a fullerene molecule. It creates Cartesian coordinates for any fullerene isomer and performs a force field optimization. It also produces fullerene graphs from Schlegel projections (C<sub>250</sub> shown here) and determines shape, volume and surface area. It is an open-source code freely available at Massey University's web-site and used by many research groups overseas, i.e. in Brazil, China, Colombia, France, Germany, Japan, India, Italy, Iran, New Zealand, Poland, Russia, Taiwan, Ukraine, United Kingdom, and the USA.*

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