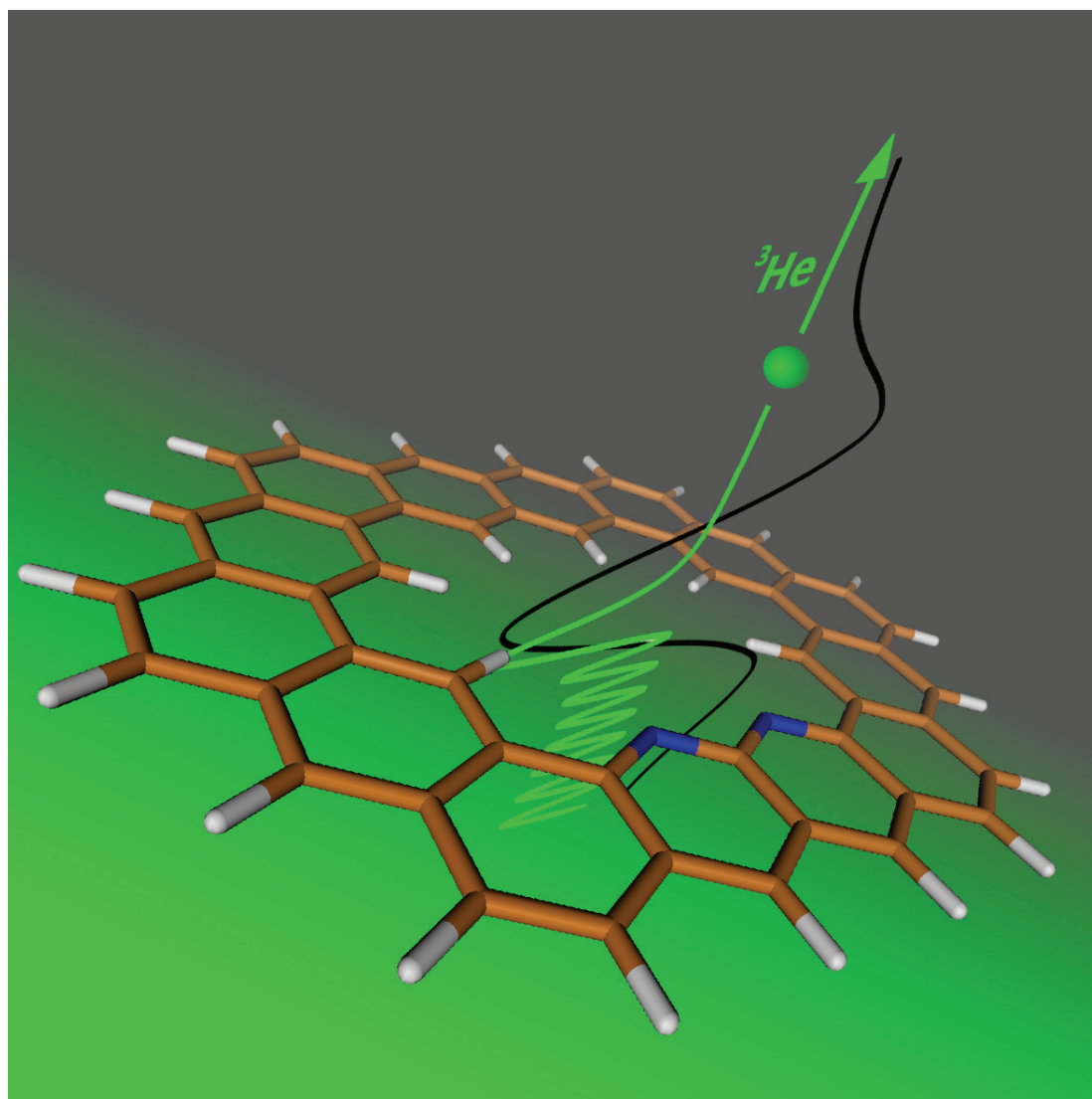

CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
NEW ZEALAND INSTITUTE FOR ADVANCED STUDY,
INSTITUTE OF NATURAL SCIENCES
and **INSTITUTE OF FUNDAMENTAL SCIENCES**
Bldg. 40 and 44, Private Bag 102 904, North Shore MSC, Auckland, New Zealand
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**2011 REPORT TO UNIVERSITY COMMERCIAL ACTIVITIES GROUP
(CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS)**



Helium going through a nanopore in graphene
(designed by Andreas Hauser)

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. All articles published are in highly acclaimed international journals of high impact factor such as the *Physical Reviews* series of journals including *Physical Review Letters*. I believe that compared to other research centres here in New Zealand, which often are larger in size than ours with greater research funding, we have achieved 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 the DAAD and the Humboldt Foundation), the 2 Marsden grants currently running in our research centre, the many high-standing international visitors who joined our centre in 2011, and the award of the Fukui Medal to Peter Schwerdtfeger. Moreover, the number of citations per year for work carried out at Massey University published since 2003 (the year our research centre was established) exceeds now 400.

Research Output: This year we published over 40 articles in top journals and books amongst 4 permanent academic staff, 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. P. Schwerdtfeger took long leaves taken over two short periods from June 3 to August 14 and September 25 to November 27 to attend international conferences and to deliver lectures at several Universities in Germany as part of the Humboldt Research Prize, and to attract potential postdoctoral fellows, PhD and MSc students. Together with P. Bowman, he was invited to the final round of Marsden, but the proposal was rejected at the end (only one chemist and one physicist in the country received a Marsden award!). Nevertheless, our research centre had 2 Marsden grants running in full in 2011 (one each by J. Brand and P. Schwerdtfeger), and 2 finished beginning of 2001. Notable achievements are that A. Borschevsky received the Helmholtz-Institute Mainz Visiting Researcher Grant, Thomas Ernst the NZIAS Postgraduate Research Excellence Award 2011, Jonas Wiebke won the young researcher poster competition at the APCTCC5 conference in Rotorua, P. Schwerdtfeger was awarded the 2011 Fukui Medal, James Avery published a book on "Symmetry Adapted Basis Sets: Automatic Generation for Problems in Chemistry and Physics", and R. Tonner and P. Schwerdtfeger were awarded the title page in PCCP for their article on the subject of biomolecular homochirality. The whole chemistry group was very active organizing the international APCTCC5 conference in Rotorua, which was a huge success with 120 international participants. The conference was sponsored by NZIAS, the German Science Foundation, and by the New Zealand – German RS&T agreement.

The Future – Opportunities, Risks and Directions: The Double-Helix Computer Cluster purchased in 2004 has now been completely replaced through Massey University's capital equipment expenditure fund and partly through an insurance claim for 40,000 NZ\$ due to damage of computer equipment from a power-cut in Albany. The computer room in Albany still requires a power back-up generator (!), but nothing has been done yet to address this problem. We pointed out last year that in financial terms, the damage caused by several recent

power cuts 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 a 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 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 research group currently carries out research in environmental sciences, addressing issues like the Pike-Mine accident and global warming, by designing efficient methods for gas separation and storage.

J. Avery, M. Wormit and A. Punnett currently administer the Double-Helix Supercomputer. J. Avery has compiled the following hard-and software overview for the Double-Helix Supercomputer: We are in the process of establishing a supercomputing environment appropriate for the heavy computational needs in our institute. The supercomputer is being built in an evolutionary fashion, as grants allow us to incrementally increase the capacity. This year, we have been able to almost triple the computing capacity of the CTCF supercomputer. We measure the computational power of the cluster using the SPEC2006fp rate, which, while still approximate, is based on real world HPC applications rather than theoretical peak performances, and which includes quantum chemical and physical applications used by our group. We have increased our capacity from 160 cores, 480 GB RAM, and approx. 3000 SPECfp, to a total of 624 CPU cores, 1.7TB RAM, and approx. 8800 SPECfp. This has been done through new purchases and consolidation of existing resources, as detailed below.

The main addition consists in a newly purchased 16 node SuperMicro system, constituting an increase of computing power by 170% (384 cores, 1TB RAM, 5000 SPECfp). They are tightly interconnected by quad data rate Infiniband (QDR IB), facilitating high-bandwidth, low latency message passing. This allows a single large-scale massively parallel computation to utilize up to all 384 cores and 1TB RAM at once, and greatly increases the efficiency of multi-node calculations in general.



We are working on consolidating the computing resources and associated system administration tasks between institutes. The computational resources of the existing BestGRID cluster run by IIMS are implemented into our new cluster, and constitutes around 7% (600 SPECfp) of the total computing power. During the first quarter of 2012, IIMS plan to migrate their remaining machines from the Zaphod cluster, constituting in total approximately 16% of our total computing power. Further consolidation of computing resources is possible: a straightforward possibility is the integration of the INS machines into the shared supercomputing environment.

We have repurposed the BestGRID file server as our head node, which serves a shared 21TB file system comprised of 16 two-terabyte disks in a striped, redundant RAID6 configuration with one spare disk. This allows failure of up to 2 disks simultaneously without interruption of service, and 3 simultaneous disk failures without data loss. The head-node runs the Bright Cluster Manager, which allows easy management of the large number of heterogeneous machines in our setup. Advanced system monitoring and early error detection gives us a high level of availability, and load and performance monitoring ensures a stable high utilization of computing resources. The head node serves disk images for all nodes, letting us reinstall or repurpose nodes in less than a minute. Disk is served to all machines over two dedicated gigabit ether-net connections, allowing peak transfer of 2Gb/s, and to our Infiniband enabled machines over IB with up to 40Gb/s.

Staffing: 2011 we saw Dr. James Avery from Copenhagen joining our research centre as a research officer to look after our hard- and software requirements. For 2012 Jane Allison, a computational biologist from the ETH Zürich, is joining our research centre to take up a position as Lecturer within INS. For further information see the attachment. There will be two new PhD students and one postdoctoral fellow joining our CTCP in 2012.

Financial: See attachment

Acknowledgment: The Director likes to thank all CTCP members for their wonderful and hard work done last year and wishes everybody a successful 2012. We enjoyed constant moral and financial support from Profs. Robert Anderson and Gaven Martin. 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: January 5, 2012

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):

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: James Avery, Kyle Beloy, Andreas Hauser, Jonas Wiebke, Michael Wormit, Mustafa Hasanbulli, Oleksandr Fialko, Andrew Punnet, Ulrich Zülicke (Palmerston North), Vesna Davidovic-Alexander, Gabriele Jaritz, and Alberto Cetoli.

Personnel:

Prof. Peter Schwerdtfeger (Director of CTCP)

Prof. Joachim Brand (Deputy Director of CTCP)

Prof. Uli Zülicke (previously based in Palmerston North, now at Victoria University of Wellington)

Dr. James Avery (Research Officer, from March 25th, 2011)

Dr. Patrick Bowman (Senior Lecturer)

Dr. Elke Pahl (Lecturer)

Honoray Members:

Dr. Matthias Lein

Dr. Tilo Söhnle

Secretaries:

Vesna Davidovic-Alexander (IAS)

Muharram Khoussainova (INS)

PhD Students:

Thomas Ernst

Mustafa Hasanbulli

Andrew Punnett

Gabriele Jaritz

MSc Students:

Jake Gulliksen

Exchange Students:

Anna-Lena Deppenmeier, Georg-August-Universität Göttingen, Bachelor Thesis: “Searching for large parity violations: Theoretical studies of penta-atomic uranium compounds” (Supervisors: P. Schwerdtfeger and A. Borschevsky)

Marie-Coralie Delattre, Universite de Lyon, France, working on Numerical solutions for Bose-Einstein condensates, March – June 2011 (Supervised by O. Fialko and J. Brand)

Ole Schumann, working on Monte-Carlo Simulation, April – June 2011 (Supervisor: E. Pahl)

Postdoctoral Fellows:

Dr. Behnam Assadollahzadeh (Marsden fellow)

Dr. Kyle Beloy (Marsden fellow)

Dr. Susan Biering (Postdoctoral fellow)

Dr. Anastasia Borschevsky (Marsden fellow)

Dr. Alberto Cetoli (Marsden fellow)

Dr. Oleksandr Fialko (Marsden fellow)

Dr. Andreas Hauser (Postdoctoral fellow)

Dr. Renyuan Liao (Massey postdoctoral fellow)

Dr. David Hallwood (Marsden fellow)

Dr. Michael Wormit (Alexander von Humboldt Feodor Lynen fellow)

Dr. Jonas Wiebke (DAAD fellow)

Visitors from other institutions:

Long Term:

Prof. Phil Bunker (NRC, Ottawa Canada)

Prof. Andreas Dreuw (University of Heidelberg)

Dr. Jacob Dunningham (University of Leeds)

Prof. Victor Flambaum (University of New South Wales)

Prof. Gernot Frenking (Philipps University Marburg)

Prof. Heinz Ggäggeler (Bern University and PSI Villigen)

Dr. Mirian Tsulaia (University of Liverpool)

Prof. Per Jensen (University Wuppertal, Germany)

Dr. Gloria Moyano (Universidad de Antioquia, Medellin, Colombia)

Short Term:

Prof. Rod Bartlett (University of Florida)

Prof. Peter Drummond (Swinburne University of Technology)

Prof. Sergej Flach (Max-Planck Dresden)

Prof. Gernot Frenking (Philipps University Marburg)

Prof. Stephen Hughes (Queens University, Canada)

Prof. Roy Johnston (University of Birmingham)

Prof. Piotr Piecuch (Michigan State University)

Prof. Robert Glaser (Ben-Gurion University of the Negev)

Dr. Mikhail Kozlov (St. Petersburg)

Dr. Florent Calvo (University of Lyon)

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
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
Quantum enhanced precision measurement
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
Variation of Fundamental Constants in Space-Time

Grants Received/Continuing:

- A. Hauser and P. Schwerdtfeger received a VC Strategic Innovation Fund of NZ\$ 25,000 for the project entitled “New Zealand’s answer to global warming: nanomaterials for methane reduction.”
- J. Brand, P. Bowman and P. Schwerdtfeger received a grant of NZ\$ 100,000 from Massey University CAPEX for the replacement of the old double-helix supercomputer.
- J. Brand: Ongoing Marsden grants on “Few-particle dynamics of ultracold atoms” (since 2008) and “Icy tornados in the quantum world: Josephson Junctions of Bose-Einstein condensates” (since 2010).
- E. Pahl: Ongoing Dumont d'Urville fellowship together with Dr. Florent Calvo, France and P. Schwerdtfeger.
- P. Schwerdtfeger had his last year Marsden grant running together with V.V.Flambaum on “The Variation of Fundamental Constants in Space and Time” (NZ\$ 780,000 in 3 years).

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 Conference on the Chemistry and Physics of the Transactinide Elements (TAN11), in Sochi, Russia.
- A. Cetoli received a postdoctoral Fellowship award from the Wenner-Gren Foundation (Sweden).
- Thomas Ernst received the NZIAS Postgraduate Research Excellence Award 2011.

- P. Schwerdtfeger received the 2010 Humboldt Research Prize at a ceremony in Bamberg Castle, March 26, 2011. The award was handed out by the President of the Humboldt Foundation, Prof. Helmut Schwarz (seen in the picture at the right). Peter also received the 2011 Fukui Medal for his achievements in quantum chemistry, in particular for the deeper understanding of quantum relativistic effects.
- Jonas Wiebke won the young researcher poster competition at the APCTCC5 conferences in Rotorua December 13).



Ongoing PhD Theses:

- M. Hasanbulli: *Atoms in Spherical Confinements*. Supervisor: P. Schwerdtfeger and B. Pavlov (started October 15).
- G. Jaritz: *Josephson dynamics in Bose-Einstein condensates*. Supervisor: J. Brand.
- A. Punnett: *How Hadrons keep their Quarks*. Supervisor: P. Bowman.

Finished PhD Theses:

- S. Biering had her oral PhD examination January 20 and successfully defended her PhD work.
- T. Ernst: *Quantum many-body dynamics of bright matter-wave solitons*. Thesis was handed in in August 2011, Thomas successfully defended his PhD work in his oral exam December 2011, which was approved by the Massey University Doctoral Research Committee in December 2011. Supervisor: J. Brand.

Lectures at Conferences / Meetings:

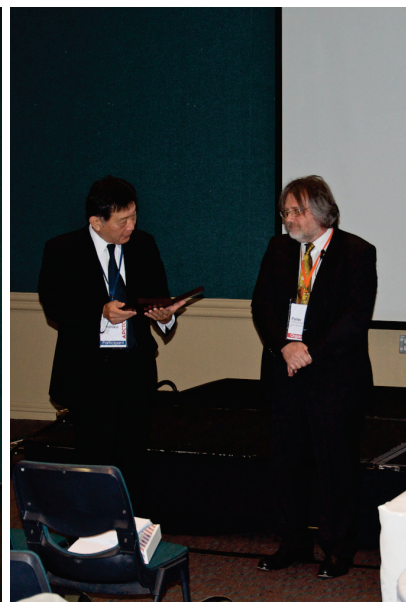
- J. Avery gave a talk entitled "*A Linear Scaling Parallel Finite Element DFT*" at APCTCC5 conference in Rotorua, New Zealand.
- K. Beloy contributed a talk at the APS March Meeting in Dallas, TX (21 – 25 Mar 2011) entitled "*Lattice-induced nonadiabatic frequency shifts in optical lattice clocks*".
- S. Biering contributed a talk at the 35th Annual Condensed Matter and Materials Meeting (Wagga Wagga 2011) in Wagga Wagga, Australia (01 – 04 Feb 2011) entitled "*Closing the gap: The influence of relativistic effects on the band structure of HgSe and HgTe*", at the New Zealand Institute of Chemistry Conference (NZIC 2011) in Hamilton, New Zealand (27 Nov – 01 Dec 2011) on "*First-principles calculations on the high-pressure phases of mercury*", and at the 5th Asian Pacific Conference of Theoretical and Computational Chemistry (APCTCC 5) in Rotorua, New Zealand (09 - 13 Dec 2011) entitled "*Relativistic effects in the solid state: The origin of the unique properties of HgX (X= S, Se, and Te)*".
- A. Borschevsky gave talks at the Fourth International Conference on the Chemistry and Physics of the Transactinide Elements (TAN11), in Sochi, Russia (*Benchmark Calculations of Atomic Properties of Element 113 to 122*), at the NZ Institute of Chemistry Conference 2011 (NZIC2011), in Hamilton, New Zealand (*Benchmark Calculations of Atomic Properties of the 7p and 8s Elements*), and at the Fifth Asian Pacific Conference of Theoretical and Computational Chemistry (APCTCC5), in Rotorua, New Zealand (*Benchmark Calculations of Atomic Properties of the 7p and 8s Elements*).
- J. Brand lectured at the Victorian Summer School in Ultracold Physics in Melbourne on "*Variational Quantum Dynamics*" and "*One-dimensional Bose gases*". He gave invited conference talks at Laser Physics 2011 in Sarajevo, Bosnia, at the Taiwan International

Workshop on Ultracold Atoms/Molecules in Hsinchu, at the Workshop of Frontiers in Ultracold Fermi gases in Trieste, Italy, at Quantum Physics with Non-Hermitian Operators in Dresden, Germany, and at the 5th Annual Dodd-Walls Symposium in Wellington.

- T. Ernst gave an invited oral presentation/tutorial on QiwiB at the VSSUP 2011 summer school at the Swinburne University of Technology in Melbourne, Australia (Jan 24 – Feb 4, 2011): “*QiwiB – Quantum integrator with interacting Bosons*”. He also gave a talk at the Dodd-Walls symposium at the University of Otago, New Zealand (Dec 6-8 2011): “*Full quantum dynamics of a bright matter-wave soliton*”.
- E. Pahl gave lectures on “*Toward the melting of mercury: A challenge to computational chemistry*” at the AMN-5 conference in Wellington (Feb. 2011), WATOC in Santiago de Compostela, Spain (June 2011), NZIC conference in Hamilton (Nov. 2011) and the APCTCC5 in Rotorua (Dec. 2011).
- Mustafa Hasanbulli gave a talk titled “*A study of confined hydrogen atom with a new confining potential*” in APCTCC-5.
- A.W. Hauser gave talks at the NZ Institute of Chemistry Conference 2011 (NZIC2011), in Hamilton, New Zealand (Nanoporous graphene – a promising new material for efficient gas separation), and at the Fifth Asian Pacific Conference of Theoretical and Computational Chemistry (APCTCC5), in Rotorua, New Zealand (*Nanoporous graphene – a two-dimensional membrane for efficient ³He/⁴He separation*). See picture above.
- P. Schwerdtfeger gave keynote lectures at several conferences: “*The Quest for Absolute Chirality*” at the NCPCHEM Meeting, Toulouse (France), January 14; The same talk was given at the AMN-5 conference in Wellington, February 11; “*Toward an accurate description of rare gas solids*”, ACS Conference, Anaheim (USA), March 30; “*From the old to the new fears: humans in the technological age*” at the Alexander von Humboldt conference on “*Angst – crippling standstill and the engine of progress*” in Graz (Austria), June 7; “*Towards the Detection of Parity Violation in Chiral Molecules*” at the WATOC conference in Santiago de Compostela (Spain), July 18; “*The Lennard-Jones potential revisited*” at the “*Symmetry in Physics*” conference at the Kloster Mehrenau in Bregenz (Austria), August 1; “*Variation of Fundamental Constants in Space-Time*” at ITAMP workshop on “*Fundamental Science with Ultracold Molecules*” at Harvard, Boston, September 30; “*High Pressure Physics – Squeezing the Hell out of Atoms*” at the *Molecular Modeling Meeting* at Heidelberg University, October 9; “*Of Spheres, Fullerenes and Hyperfullerenes*”, at the NZIC conference in Hamilton, December 1; “*Beyond the Standard Model – The Variation of Fundamental Constants in Space-Time*” at the APCTCC5 conference in Rotorua, December 13.
- M. Wormit presented a talk at the 14th Biennial Meeting of von Humboldt Fellows in Sydney (30th September-2nd October 2011): “*Colour in nature – why do plants have green leaves? A theoretical perspective.*”. He also presented a talk at the 5th Asian-Pacific Conference of Theoretical and Computational Chemistry in Rotorua (9th December-13th December 2011): “*An Efficient Parallel Tensor Algebra Library for Easy Development of Electronic Structure Methods like CC or ADC*”.
- U. Zuelicke gave invited talks at the 2012 Gordon Godfrey Workshop on Spins and Strong Correlations (Sydney, Australia, 24 – 28 October 2011): “*Mesoscopic and many-particle effects from valence-band mixing in hole nanostructures*”, and at the 14th Manawatu-Wellington Applied Mathematics Meeting (Gracefield, New Zealand, 8 November 2012): “*Quantum spintronics based on spin-orbit coupling of charge carriers*”. He also presented a contributed talk at the 5th International Conference on Advanced Materials and Nanotechnology (AMN 5, Wellington, New Zealand, 7 – 11 February 2011): “*Trigonal band structure of graphene*”.



Participants of the international *Asian-Pacific Conference on Theoretical and Computational Chemistry*, December 9-13 in Rotorua, organized by Elke Pahl (Chair), Anastasia Borschevsky, Mustafa Hasanbulli, Elke Pahl, Peter Schwerdtfeger, Jonas Wiebke, Michael Wormit, and Vesna Davidovic-Alexander.



APCTCC conference in Rotorua from the left to the right: Opening speech by Prof. Gaven Martin (HOI INS and NZIAS), plenary lecture given by Prof. Rod Bartlett (Florida, Board member of NZIAS), and award of the Fukui Medal to P. Schwerdtfeger by the president of the APATCC association Prof. Kimihiko Hirao (Japan).

Seminars and Talks:

- J. Brand gave an invited seminar talk on “*Nonlinear and Quantum Dynamics with Ultracold Atoms*”, 27 April 2011, at the National Changhua University of Education in Taiwan.
- T. Ernst gave a talk entitled “*Full quantum dynamics of a scattered soliton*”, March 25 2011, CTCP, Massey University Auckland, New Zealand.
- Mustafa Hasanbulli gave a seminar as a part of his confirmation examination titled “*A study of confined hydrogen atom with a new confining potential*” on September 23, 2011, CTCP, Massey University Albany.
- E. Pahl gave a seminar on *Cluster melting* at Victoria University Wellington (9/9/2011).
- P. Schwerdtfeger gave several talks at universities: “*The Quest for Absolute Chirality*” at the Laboratoire de Chimie et Theorique, Université de Paris 6 & CNRS (France), January 10; The same talk was given at the Université Lyon, January 20, and at CNRS in Grenoble, January 24; “*The Chemistry and Physics of Superheavy Elements*”, Cornell University (USA), January 31; “*The Origin of Biomolecular Homochirality*”, Victoria University, Wellington, April 13; “*High Pressure Physics – Squeezing the Hell out of Atoms*” at the Philipps University Marburg, June 14; “*Relativistic Pseudopotentials*” at the University of Darmstadt, June 22; “*High Pressure Physics – Squeezing the Hell out of Atoms*” at the TU Berlin, June 30; “*The Origin of Biomolecular Homochirality*”, Heidelberg University, July 11; “*From small clusters to the liquid and solid state*”, Bayreuth University, July 27; “*Beyond the Standard Model – The Variation of Fundamental Constants in Space-Time*”, Otago University, September 5; “*Beyond the Standard Model – The Variation of Fundamental Constants in Space-Time*”, Heidelberg University, October 12; Same talk at the Free University of Berlin, October 19; “*The Quest for Absolute Chirality*”, GdCH lecture organized by the German Chemical Society at the Bielefeld University, October 27; “*The Pseudopotential Approximation*” next day at the same university; “*The Quest for Absolute Chirality*” at Giessen University, November 1; “*The Elusive Chromium Dihalide Structures - A Combined Computational and Gas Phase Electron Diffraction Study*” at Frankfurt University, November 2; “*Relativistic Effects in the Chemistry and Physics of Gold*” at the Technical University of Berlin, November 9; “*Towards the Detection of Parity Violation in Chiral Molecules*” at the Fritz-Haber Institute in Berlin, November 11; on “*High Pressure Physics – Squeezing the Hell out of Atoms*” at the Karlsruhe Institute of Technology of Karlsruhe University, November 21; “*The Origin of Biomolecular Homochirality*”, GdCH lecture organized by the German Chemical Society at Darmstadt University.
- M. Wormit visited the theoretical chemistry group of the Institute of Scientific Computing at the University of Heidelberg and gave a seminar on “*Implementation of ADC using the new tensor library*”.
- U. Zuehlcke presented an invited seminar talk at IRL on 10 June, entitled “*After the prize: Graphene continues to surprise*”, and a colloquium-style talk with the same title for the University of the Third Age in Palmerston North on 21 October.

Posters:

- A. Borschevsky presented a poster at the Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC2011), Santiago De Compostela, Spain: *Benchmark Calculations of Atomic Properties of Elements 113 to 122*.
- A.W. Hauser presented a poster at the Fifth International Conference on Advanced Materials and Nanotechnology (AMN-5), Wellington, New Zealand: *Accidental conical intersections in mixed trimers of potassium and rubidium: A vibronic analysis of the 4B2 and 3A1 states*.
- J. Wiebke: “*A Fourth-Order Ab Initio Virial Equation Of State for Argon – Revisited*”

NZIC, Nov. 2011, Hamilton, NZ; APCTCC-5, Dec. 2012, Rotorua, NZ.

- M. Wormit presented a poster at the NZIC Conference in Hamilton (27th November-1st December): *"Implementation of Adc(2) for the Calculation of Electronic Excited States Using a Newly Developed Parallel Tensor Algebra Library"*
- U. Zuelicke presented a poster at the 19th International Conference on Electronic Properties of Two-dimensional Systems (EP2DS-19, Tallahassee, Florida, USA, 25 – 29 July 2011): *"Graphene's cornucopia of novel electronic effects enlarged: Results from a symmetry analysis"*.

Teaching:

- P. Bowman taught parts of 124.101 and 124.102, stage 1 physics, and was paper coordinator for 124.129 Astronomy.
- J. Brand taught parts of 124.101 and 124.102, stage 1 physics and part of 124.129 Astronomy.
- S. Biering taught the Physics Short Course, 124.011, which was held in semester 2 for the first time.
- E. Pahl taught 124.011, Foundation Studies Physics at the summer school. and 124.111, Physics for Life Sciences and was paper coordinator for the 124.111 paper, Albany offering. She designed the new (shortened) Study Guide for the Physics Short Course, 124.011 which was held in S2 for the first time (taught by Susan Biering).
- P. Schwerdtfeger taught part of stage 2 physics (124.102) thermodynamics. He also gave a lecture course on theoretical chemistry at the Philipps University of Marburg.
- Five postdoctoral fellows (S. Biering, A. Borschevsky, O. Fialko, A.W. Hauser, J. Wiebke) and all PhD students contributed teaching in the chemistry labs, physics stage 1 teaching labs and astronomy labs.

Other activities:

Papers refereed:

- J. Avery refereed a paper for Appl. Math. Lett.
- K. Beloy refereed a paper for Phys. Rev. Lett.
- P. Bowman refereed a paper for Phys. Rev. Lett. and Phys. Rev. D.
- S. Biering refereed a paper for Phys. Chem. Minerals.
- J. Brand refereed in 2011 for Phys. Rev. Lett., Phys. Rev. A and E, Europhys. Lett., Europhys. J. D, J. Phys. B, Frontiers of Physics, Phys. Lett. A, Annalen der Physik.
- Mustafa Hasanbulli refereed 2 papers for Mathematica Slovaca and Mathematical Communications.
- P. Schwerdtfeger refereed in total 78 papers 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.
- U. Zuelicke served as referee for papers submitted to Nature Communications, Phys. Rev. Lett., Phys. Rev. B, and Eur. Phys. Lett.

PhD and MSc theses refereed:

- P. Bowman was internal examiner for the PhD thesis of Thomas Ernst.
- J. Brand was examiner for the PhD thesis of Brian Wild, University of Otago and was a thesis assessor for an MSc thesis at the University of Auckland.
- E. Pahl: External New Zealand referee for PhD thesis by Sione Paea (Victoria University, Wellington – supervisor: Prof. S. Hendy).

- P. Schwerdtfeger refereed three PhD theses in 2011: a) Philip McGill (Auckland University, Supervisors: Hicham Idriss and Tilo Söhnle) on “Theoretical Studies of Model Molecule Adsorption to the Surfaces of Titania and Ruthenium”; b) Doreen Mollenhauer (Free University Berlin, Supervisor: Beate Paulus) on “Quantenchemische Untersuchungen zur Wechselwirkung von Pyridinderivaten mit Goldnanopartikeln auf Graphit- und Goldoberflächen”; c) Moritz Hopfgarten (Philipps University Marburg, Supervisor: Gernot Frenking) on “Die chemische Bindung in hochkoordinierten Übergangsmetallverbindungen”.

Conference Organisation:

- A. Borschevsky, M. Hassanbuli, J. Wiebke and M. Wormit acted as co-organizers of the APCTCC-5 conference in Rotorua.
- E. Pahl was the main organizer of the APCTCC-5 conference (120 participants from 21 countries) held in Rotorua New Zealand, December 9-13, 2011.
- P. Schwerdtfeger acted as chair for the APCTCC-5 conference in Rotorua.

Chairs at Conferences:

- J. Brand chaired sessions at Laser Physics 2011 in Sarajevo, Bosnia, at the Taiwan International Workshop on Ultracold Atoms/Molecules in Hsinchu, at the Workshop of Frontiers in Ultracold Fermi gases in Trieste, Italy, and at the 6th Annual Dodd-Walls Symposium in Dunedin.
- E. Pahl chaired Cluster session at APCTCC-5, December 10, 2011.
- P. Schwerdtfeger chaired sessions at the *Molecular Modeling Meeting* at Heidelberg University, October 9, at the NZIC conference in Hamilton, November 29, and at the APCTCC-5 conference in Rotorua, December 9.
- U. Zuehlke chaired a session at the AMN-5 conference in Wellington.

Editorial Boards / Professional Societies:

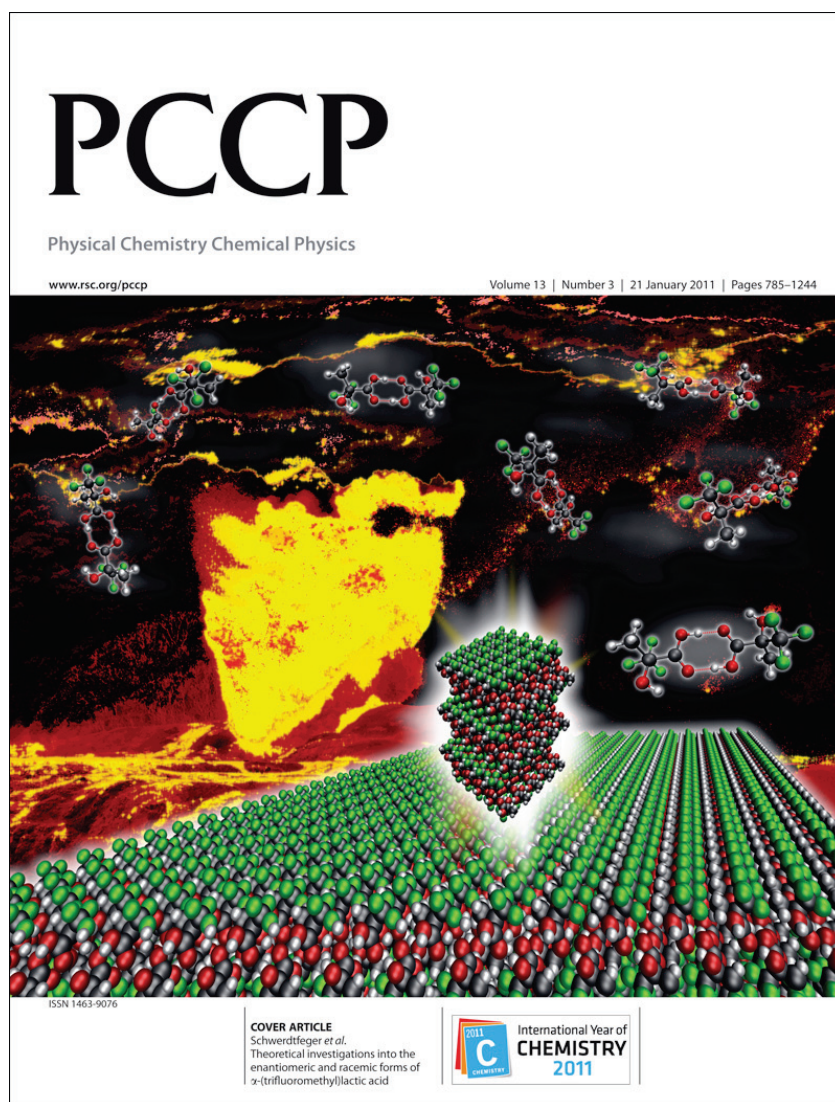
- J. Brand represented the New Zealand Association of von Humboldt Fellows as its Vice President at the Biannual Meeting of the Australian Association of von Humboldt Fellows in Sydney.
- P. Schwerdtfeger served on the editorial board for Journal of Computational Chemistry, Journal of Computational Methods in Sciences and Engineering, and Wiley Interdisciplinary Reviews: Computational Molecular Science. He also served as the President of the New Zealand Humboldt Association, for the election of the Rutherford Medallist (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:

- S. Biering delivered two lectures to year 13 students at Orewa and Long Bay College.
- P. Bowman delivered lectures to year 13 students at Whangaparaoa, Mahurangi and Glenfield Colleges. Bowman also delivered a physics masterclass to year 13 students.
- J. Brand delivered a masterclass in Physics to year 13 high school students.
- E. Pahl was invited to give a seminar on Quantum Physics at the New Zealand Association for Gifted Children conference for gifted teens in March 2012.
- P. Schwerdtfeger gave a public lecture at the Wellington law school organized by the NZIC as a “Year of Chemistry” talk on “*Beyond the Periodic Table – Going for the Superheavy Elements*”, April 13. He also gave a public lecture at the University of Ulm on “*Relativity and the Chemistry of Gold*”, before the award ceremony for the top chemistry. He also gave a speech on July 4 for the launch of a new book edited by Prof. Dietmar Goldschmidt, for which I contributed a chapter (P. Schwerdtfeger, “*Von der absoluten zur*

relativen Zeit – Die Zeit im Wandel der Zeit”, in *Phänomen Zeit – Dimensionen und Strukturen in Kultur und Wissenschaft*, ed. Dietmar Goltschnigg, Stauffenberg Verlag, Tübingen. He also took part in a chemistry masterclass for school children organized by Massey University Auckland and gave a talk on “*Beyond the Periodic Table – Going for the Superheavy Elements*”, September 21.

- U. Zuelicke gave a presentation “*Physical principles of nanoscience*” to Year-12 high-school students as part of *Nanocamp 2011* (Palmerston North, 17 – 21 January 2011). He also presented a lecture entitled “*Quantum nanoscience*” at the 2011 Physics Teachers Picnic at Victoria University of Wellington (22 November 2011).



R. Tonner, V. A. Soloshonok, P. Schwerdtfeger, “Theoretical investigations into the enantiomeric and racemic forms of α -(trifluoromethyl)lactic acid”, *Phys. Chem. Chem. Phys.* 13, 811-817 (2011). (*invited article special issue on biomolecular homochirality*).

PUBLISHED WORK

Articles published in 2011 refereed journals:

1. J. Avery, J. Avery, "Sturmians and Generalized Sturmians in Quantum Theory", *Structure and Bonding* **999**, (2011), 47 pages. (DOI: 10.1007/430_2011_53).
2. R. Bast, A. Koers, A. S. P. Gomes, M. Iliaš, L. Visscher, P. Schwerdtfeger, T. Saue, "Analysis of parity-violation in chiral molecules", *Phys. Chem. Chem. Phys.* **13**, 864-876 (2011).
3. K. Beloy, "Lattice-induced nonadiabatic frequency shifts in optical lattice clocks", *Phys. Rev. A* **82**, 031402(R)-1-4 (2010); (not listed last year due to late appearance).
4. K. Beloy, A. Borschevsky, V. V. Flambaum, P. Schwerdtfeger, "Effect of α -variation on a prospective experiment to detect variation of m_e/m_p in diatomic molecules", *Phys. Rev. A* **84**, 042117-1-5 (2011).
5. K. Beloy, M. G. Kozlov, A. Borschevsky, A. Hauser, V. V. Flambaum, P. Schwerdtfeger, "Rotational Spectrum of molecular ion NH^+ as a probe for α - and m_e/m_p -variation", *Phys. Rev. A* **83**, 062514-1-7 (2011).
6. K. Beloy, A. W. Hauser, A. Borschevsky, V. V. Flambaum, P. Schwerdtfeger, "Effect of α -variation on the vibrational spectrum of Sr_2 ", *Phys. Rev. A* **84**, 062114-1-4 (2011).
7. S. Biering, P. Schwerdtfeger, "High-pressure transitions in bulk mercury: A density functional study", *Theoret. Chem. Acc.* **130**, 455-462 (2011). (invited article for the *Nagase Festschrift*).
8. A. Borschevsky, K. Beloy, V. V. Flambaum, P. Schwerdtfeger, "Sensitivity to α -variation in ultracold atomic-scattering experiments", *Phys. Rev. A* **83**, 052706-1-5 (2011).
9. A. Borschevsky, T. Zelovich, E. Eliav, and U. Kaldor "Precision of calculated static polarizabilities: Ga, In and Tl atoms", *Chem. Phys.*, published online (10.1016/j.chemphys.2011.05.011) (2011).
10. P.O. Bowman, K. Langfeld, D.B. Leinweber, A. Sternbeck, L. von Smekal, A.G. Williams, "Role of center vortices in chiral symmetry breaking in SU(3) gauge theories", *Phys. Rev. D* **84**, 034501-1-9 (2011).
11. V. A. Dzuba, V. V. Flambaum, K. Beloy, A. Derevianko, "Hyperfine-mediated static polarizabilities of monovalent atoms and ions", *Phys. Rev. A* **82**, 062513-1-6 (2010); (not listed last year due to late appearance).
12. T. Ernst, D. W. Hallwood, J. Gulliksen, H.-D. Meyer, and J. Brand, "Simulating strongly correlated multiparticle systems in a truncated Hilbert space", *Phys. Rev. A* **84**, 023623-1-8 (2011).
13. D. Futterer, M. Governale, U. Zülicke, J. König, "Band-mixing-mediated Andreev reflection of semiconductor holes", *Phys. Rev. B* **84**, 104526:1-7 (2011).
14. C. Giese, F. Stienkemeier, M. Mudrich, A.W. Hauser, and W.E. Ernst, "Homo- and heteronuclear alkali metal trimers formed on helium nanodroplets. part II. femtosecond spectroscopy and spectra assignments", *Phys. Chem. Chem. Phys.* **13**, 18769-18780, (2011).
15. D. W. Hallwood, J. Brand "Engineering mesoscopic superpositions of superfluid flow", *Phys. Rev. A* **84**, 043620-1-9 (2011).
16. A.W. Hauser and W.E. Ernst, "Homo- and heteronuclear alkali metal trimers formed on helium nanodroplets. part I. vibronic spectra simulations based on ab initio calculations", *Phys. Chem. Chem. Phys.* **13**, 18762-18768 (2011).
17. A. Hermann, P. Schwerdtfeger, "Opening of the UV-window for water under pressure", *Phys. Rev. Lett.* **106**, 187403-1-4 (2011).

18. M. Jääskeläinen, M. Lombard, U. Zülicke, "Refraction in spacetime", *Am. J. Phys.* **79**, 672-677 (2011).
19. R. Keyzers, P. G. K. Clark, M. Lein, *Org. Biomol. Chem.* 2011 (DOI: 10.1039/C2OB06926A).
20. T. Kernreiter, M. Governale, A. R. Hamilton, U. Zülicke, "Charge transport by modulating spin-orbit gauge fields for quasi-one-dimensional holes" *Appl. Phys. Lett.* **98**, 152101:1–3 (2011). selected for Virtual Journal of Nanoscale Science & Technology
21. M. Lein, J. A. Harrison, "Highly Fluxional [Y(C(SiH(CH₃)₂)₃)₃]: A DFT Characterization of Structure and NMR Spectra", *J. Chem. Theory Comput.* **7**, 385-389 (2011).
22. M. Lein, J. A. Harrison, A.J. Nielson, "M...H–Si interactions in [{M(CpSiMe₂H)Cl₃}₂], (M = Zr, Hf, Ti and Mo) complexes", *Dalton Trans.* **40**, 10731-10741 (2001).
23. R. Liao and J. Brand, "Travelling dark solitons in superfluid Fermi gases", *Phys. Rev. A* **82**, 041604-1-4 (2011).
24. A. P. Micolich, U. Zülicke, "Tracking the energies of one-dimensional sub-band edges in quantum point contacts using dc conductance measurements", *J. Phys.: Condens. Matter* **23**, 362201:1–8 (2011).
25. B. Ostojić, P. R. Bunker, P. Schwerdtfeger, B. Assadollahzadeh, P. Jensen, "The predicted infrared spectrum of the hypermetallic molecule MgOMg in its X ¹Σ_g⁺ and \tilde{a} ³Σ_u⁺ electronic states", *Phys. Chem. Chem. Phys.* **13**, 7546-7553 (2011).
26. E. Pahl, D. Figgen, A. Borschevsky, K. A. Peterson, P. Schwerdtfeger, "Accurate potential energy curves for the group IIB dimers, Zn₂, Cd₂, and Hg₂", *Theoret. Chem. Acc.* **129**, 651-656 (2011). (*Pyykkö Festschrift*).
27. V. Pershina, A. Borschevsky, and J. Anton, "Fully Relativistic Study of Intermetallic Dimers of Group-1 Elements K through Element 119 and Prediction of their Adsorption on Noble Metal Surfaces", *Chem. Phys.*, published online (doi:10.1016/j.chemphys.2011.04.017) (2011).
28. D.S. Roberts, P.O. Bowman, W. Kamleh, D.B. Leinweber, "Wave Functions of the Proton Ground State in the Presence of a Uniform Magnetic Field in Lattice QCD", *Phys. Rev. D* **83**, 094504-1-15 (2011).
29. P. Schwerdtfeger, "In the Year of Chemistry: From Mendeleev to Albert Einstein – The Periodic Table of the Elements and Beyond", *ChemNZ*, *April issue*, 91-95 (2011). (*invited article for the Year of Chemistry*).
30. P. Schwerdtfeger, "The Pseudopotential Approximation in Electronic Structure Theory", *Chem. Phys. Chem.* **12**, 3143-3155 (2011). (*invited article for the special issue on Recent Progress in Theoretical and Computational Chemistry*).
31. P. Schwerdtfeger, B. Assadollahzadeh, J. R. Cheeseman, U. Rohrmann, R. Schäfer, "The accuracy of the pseudopotential approximation for magnetizabilities and electric multipole moments", *J. Chem. Phys.* **134**, 204102-1-11 (2011).
32. S. Kim, J. Brand, "Decay modes of two repulsively interacting bosons", *J. Phys. B – At. Mol. Opt. Phys.* **44**, 195301-1-10 (2011).
33. R. Tonner, G. Frenking, M. Lein, P. Schwerdtfeger, "Packed to the Rafters – Filling up C₆₀ with Rare Gas Atoms", *Chem. Phys. Chem.* **12**, 2081-2084 (2011).
34. J. Wiebke, P. Schwerdtfeger, G. E. Moyano, E. Pahl, "An Atomistic Fourth-Order Virial Equation of State for Argon from First Principles Calculations", *Chem. Phys. Lett.* **514**, 164-167 (2011).
35. R. Tonner, V. A. Soloshonok, P. Schwerdtfeger, "Theoretical investigations into the enantiomeric and racemic forms of α-(trifluoromethyl)lactic acid", *Phys. Chem. Chem. Phys.* **13**, 811-817 (2011). (*invited article special issue on biomolecular homochirality*).
36. R. Tonner, V. A. Soloshonok, P. Schwerdtfeger, "Reply to Comment on 'Theoretical investigations into the enantiomeric and racemic forms of α-(trifluoromethyl)lactic acid' by M. A. Suhm and M. Albrecht, *Phys. Chem. Chem. Phys.* 2011, 13, 4159-4160.", *Phys. Chem. Chem. Phys.* **13**, 4161-4162 (2011).

Refereed Conference Proceedings:

37. D.S. Roberts, P.O. Bowman, W. Kamleh, D.B. Leinweber, "Proton wave functions in a uniform magnetic field", *AIP Conf. Proc.* **1354**, 224 (2011).

Books:

38. J. Avery, S. Rettrup, and J. Avery: "Symmetry-Adapted Basis Sets: Automatic Generation for Problems in Chemistry and Physics". World Scientific, October 2011, ISBN: 978-981-4350-46-4, 240pp.

Chapters in Books:

39. P. Schwerdtfeger, "Von der absoluten zur relativen Zeit – Die Zeit im Wandel der Zeit", in *Phänomen Zeit – Dimensionen und Strukturen in Kultur und Wissenschaft*, ed. Dietmar Goltschnigg, Stauffenberg Verlag, Tübingen (2011); p.41-45.
40. J. Avery and J. Avery, "The Generalized Sturmian Method", Chapter 6 in "Solving the Schrödinger Equation: Has Everything Been Tried?", ed. Paul Popelier, Imperial College Press, November 2011, ISBN: 978-1-84816-724-7; p.111-139.

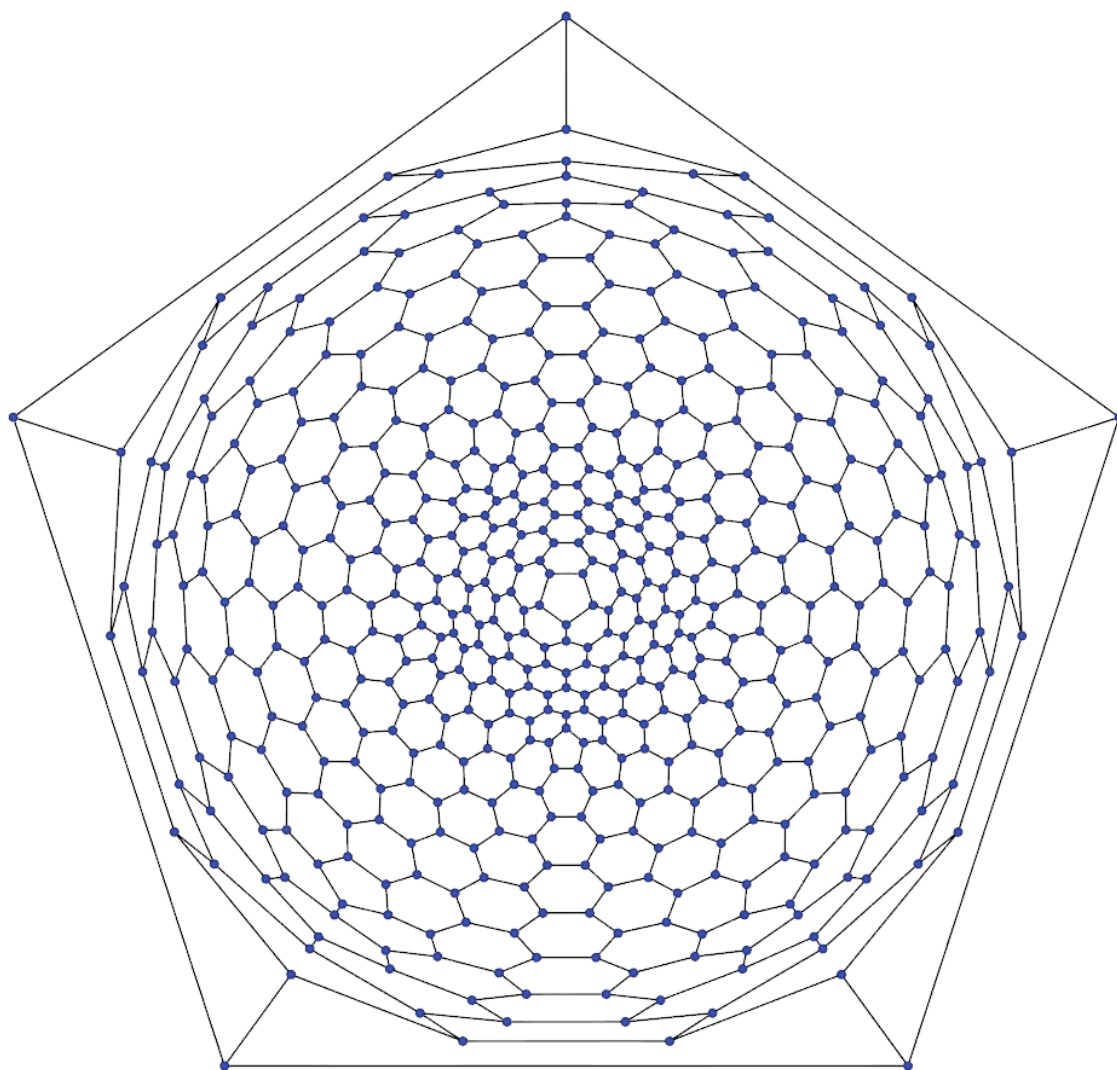
Archives:

41. A. Borschevsky, M. Ilias, V.A. Dzuba, K. Beloy, V.V. Flambaum, P. Schwerdtfeger, Relativistic ab initio calculations of the P-odd interaction constant W_A in diatomic molecules, arXiv:submit/0389593.
42. R. G. Scott, F. Dalfovo, L. P. Pitaevskii, S. Stringari, O. Fialko, R. Liao, J. Brand, "The decay and collisions of dark solitons in superfluid Fermi gases", arxiv:1109.6444
43. J. J. Cooper, D.W. Hallwood, J.A. Dunningham, J. Brand, "Robust Heisenberg limited measurements in a multimode interferometer", arXiv:1101.3852
44. A. Yu. Cherny, J.-S. Caux, J. Brand, "Theory of superfluidity and drag force in the one-dimensional Bose gas", arXiv:1106.6329
45. O. Fialko, A. S. Bradley, J. Brand, "Quantum tunneling of a vortex between two pinning potentials", arXiv:1105.5869, to appear in *Phys. Rev. Lett.*

Software developments:

- T. Ernst: Software package *Qiwib* available under an open source license and can be found online at qiwib.googlepages.com
- P. Schwerdtfeger: Software package Fullerene 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>
- J. Avery: Software package *The Generalized Sturmian Library* available as open source and can be found online at sturmian.kvante.org.
- J. Avery: Software package *libspace*, a library supporting finite element methods in quantum chemistry, available as open source and can be found online at libspace.kvante.org.

- J. Avery: Software package *libintegral*, a library supporting fast multi-center electron repulsion integrals of exponential type orbitals, available as open source and can be found online at libintegral.kvante.org.
- J. Avery: Software package *Pauling*, a set of programs for rapid automatic generation of symmetry-adapted many-electron basis functions; not yet online.



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_{540} shown here) and determines shape, volume and surface area. It is a open-source code freely available at Massey University's web-site and used by many research groups overseas.