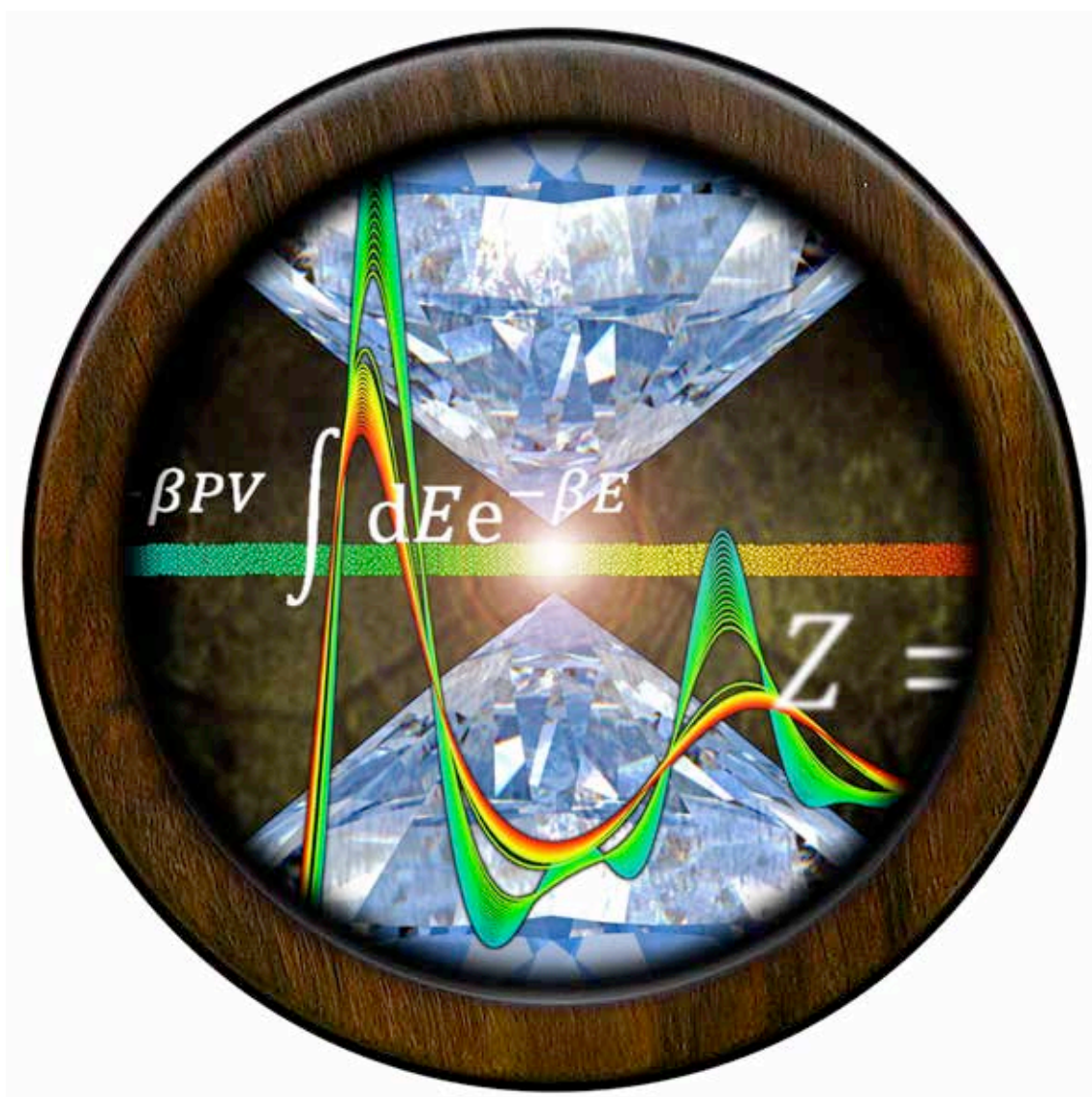

CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
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2013 MASSEY UNIVERSITY ANNUAL REPORT CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS



A glimpse into high-pressure phase transitions: The importance of a quantitative understanding of solid-liquid transitions under high pressure is contrasted by the extreme difficulties of Diamond-Anvil Cell experiments at these conditions. Here, quantum theory enables accurate Monte Carlo simulations of melting of argon under pressures up to 100 GPa that can challenge such experiments (picture designed by J. Wiebke).

Objectives of Research Centre: *Our objective is to advance and disseminate knowledge in the area of theoretical/computational chemistry and physics, and to maintain high international standards in this research field only matched by top research institutes world-wide.*

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, and our articles appear regularly in top journals such as *Physical Review Letters* or *Angewandte Chemie*. The many high-standing international visitors who joined our centre in 2013, and the many invitations to international conferences received by our staff are a clear indication of our success. Our research centre is unique within New Zealand and perhaps the wider Australasian area.

Research Output: This year we published 41 articles in journals and books (a large number in top journals) amongst 8 permanent academic staff, again a truly exceptional year for our research centre. 2013 highlights were papers published in *Nature*, *Nature Chemistry*, *Physical Review Letters* and *Angewandte Chemie*. See the attached list of publications for more details.

Activities and achievements: All members of CTCP were involved in chemistry, physics or biology teaching as outlined in the Appendix 4. 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. Amongst the outstanding achievements were awards of two Marsden grants – a fast-start Marsden grant for Jane Allison and a full Marsden grant for J. Brand (together with Otago University) – and the Massey University Women Award for Elke Pahl. The large number of international eminent visitors we get each year clearly underlines our international visibility and achievements.

The Future - Opportunities, Risks and Directions: We are a top research centre of international exceptional high standing; however, the support in terms of PhD students and postdoctoral fellows is quite tiny compared to international standards. Our exceptional productivity comes from our diligently determined and hard working staff striving beyond their best within the financial means available. Our tack yet wears thin, and we require far better support and more serious commitments, specifically in terms of PhD students and postdoctoral fellows. The recent major in chemistry (with only a minor in physics) has become a challenge for our stretched working hours, detracting greatly from the pure research for which our centre was intended. The risks here are clear: continued unchecked, there will be a downturn in research productivity and international vital collaborations. One quick-fix solution is obvious: an increase in Marsden proposals for 2014/15. However, due to our past wins, these have become increasingly more difficult for our centre to achieve. We however do realize that our external financial income needs to be improved substantially for 2015.

Our research institute additionally requires a high-performance compute cluster (HPCC) system, which in comparison to other laboratory apparati, is relatively low-cost. It cannot be overstressed that this is not a novelty or luxury – it is a requirement. In order to remain competitive against other centres worldwide, large-scale parallel computations must be carried out in as rapid and efficient manner as possible. Such computations span multiply

disconnected research areas – from fundamental physics to applied biochemistry. Ergo, we are most eager to maintain and refurbish our computational facilities. In 2013, we applied for capital equipment funding to replace old computer nodes, which had exceeded their expected lifetime after being active for more than four years. After a rejection, we were informed by the College of Sciences regarding our eligibility to upgrade our HPCC over the forthcoming four years, with a financial input of one million NZ\$. This is ecstatic news, and shall help us tremendously in our future research plans; especially in easing the heavy burdens on the currently over-subscribed HPCC. Our policy was, is, and shall remain so – that our HPCC is open to any active research group at Massey University (regardless of NZIAS or CTCP affiliations). Once our upgrades are underway, many more computationally active research groups at Massey will join in the profit, continuing to enhance Massey's reputation for research and performance.

Work in progress: There are too many research projects in progress to list all of them (see attachment for more details). Funding in 2014 is anticipated mainly through Marsden Grants (see appendix 1). A 250,000\$ grant by Massey University College of Science will be used to maintain and upgrade our current Double-Helix Supercomputer cluster in 2014.

Staffing: 2013 saw the addition of our new research officer, Joshua Bodyfelt, who will be responsible for maintaining our compute cluster.

Financial: See Appendix 4.

Acknowledgment: The Director is grateful to all CTCP members for their (again) outstanding performance and very hard work in 2013, and wishes everybody a (even more) successful 2014. We enjoyed constant moral and financial support from Profs. Robert Anderson, Brigid Heywood and Gaven Martin. 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: January 31, 2014

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 1

Research Objectives for 2014

- J. R. Allison will begin the work funded by her recent Marsden Fast Start grant, namely the development of coarse-grained lipid models en route to the development of a multi-scale model for biomolecular simulation, together with Sereina Riniker at the ETH Zurich. A new PhD student, Elisey Kobzev, funded by a Commonwealth Scholarship, has already begun work on this project, and the search for another, funded by the Marsden grant, is under way. A third PhD student, Ashar Malik, will arrive as soon as a visa is obtained to work on combining molecular dynamics (MD) simulations with new structure-based methods for inferring phylogenetic relationships together with Anthony Poole at the University of Canterbury. Jane will be putting together an NIH grant with David Liberles (University of Wyoming) on a similar topic. A. Poole and Jane are also close to publishing their work on the p19 viral suppressor protein. She will continue her research on combining NMR data with MD simulations in collaboration with Lorna Smith at the University of Oxford, which is partly carried out by CTCP PhD student Lukas Wirz. Several publications on this topic are expected shortly. She will also continue to work with Jack Flanagan at the Auckland Cancer Research Institute to investigate the structural and dynamic effects of oncogenic mutations to PI3K α , with the ultimate aim of developing new drugs. The MSc student working on this project, William Irvine, is expected to finish in March. Finally, Jane will continue her involvement in the research of INMS staff members Xue-Xian Zhang and Evelyn Sattlegger, and will be looking to publish the outcomes of her advisory role with PhD student Davoud Zare (supervisor: Prof. Kate McGrath, Victoria University) and her co-supervision of PhD student Tatyana Pichugina (supervisor: Justin O'Sullivan, Liggins Institute), who are working in the areas of materials science and genome modelling, respectively.
- J. D. Bodyfelt: In 2014, his professional goals are: (1) Put into action fully and supervise the Marvin HPCC upgrade; this includes procurement, installation, pre-deployment testing, and operational deployment announcement. (2) Obtain a Marsden Fast Start grant, in order to fund and manage his own PhD students. Also, continued inquiry into NZIAS PhD Scholarship opportunities and NZ-external grant possibilities. In the winter months, host a M.S. exchange student from Uppsala University who intends to continue her PhD (with Bodyfelt as advisor) starting in 2015. (3) Continue his annual personal aim for ten publications in impacting international journals. Disseminate his findings at a minimum of two international physics conferences (APS and SIAM 2014 annual meetings). (4) Continue growing an Oceania research network by reaching out to, and establishing collaboration paths with, members at Tata Institute of Fundamental Research (India), University of Auckland (NZ), Nanyang Technological University (Singapore), and RIKEN Center for Advanced Photonics (Japan).
- P. Bowman is working on testing the "Abelian dominance" model of quark confinement through first-principles Lattice QCD simulations. He is also developing Lattice simulations of QED to explore the regime of very strong electric fields (such as in heavy atomic nuclei).
- J. Brand will continue his research in the area of quantum phenomena and nonlinear waves in quantum gases. A particular goal is establishing a route toward the emulation of problems in relativistic field theory with ultra-cold atomic gas experiments. In this context, his research group will study bubble nucleation by quantum tunnelling, which has relevance in various fields of physics including the early universe and liquid helium

mixtures. Another focus of research is related to the Marsden funded collaboration with the Mikkel Anderson (UoO) on the experimental and theoretical study of few-body dynamics of ultra-cold atoms. During the year he will compete for additional Marsden funding and continue his involvement as a theme leader in the CoRE bid of the Dodd-Walls Centre for Photonic and Quantum Technologies. Two new PhD students (Jayson Cosme and Sophie Shamailov) are expected to start working on their research projects in the beginning of the new year. Prof. Brand is further involved in organizing (and will be lecturing at) a Graduate Summer School (VSSUP-2014) in Melbourne and in the upcoming NZIAS/MPIPKS Tandem Workshop *Nonlinear Physics at the Nanoscale: A Cross-Fertilization on Stochastic Methods*.

- S. Flach will 1) compete for a Marsden grant; 2) expand the research collaboration with Yu. Kivshar's centre at ANU Canberra (Australia), B. Altshuler at Columbia U NY (USA), D. Campbell at Boston U (USA), M. Ivanchenko's group at U Nizhnii Novgorod (Russia), L. Morales-Molina and R. Vicencio at U Santiago (Chile), T. Bountis at U Patras (Greece), G. Tsironis at U Crete (Greece); 3) coordinate the first Tandem Workshop meeting MPIPKS-NZIAS in Dresden (Germany), and prepare the return meeting in NZ; 4) coordinate, after the successful first Christmas symposium on the physics of complex systems, a second symposium by the end of 2014.
- E. Pahl: In 2014, she wants to: (1) Continue and strengthen her research activities on the field of *melting simulations* of weakly interacting systems. The focus will be on (a) high-pressure studies of rare gas clusters – tackling the fundamental problem of how to determine the volume of small clusters (subject of the Massey woman award) and extending previous high-pressure studies on solid Argon to heavier rare gases; (b) intensify the program development to study molecular systems like nitrogen; (c) extending the mercury melting studies to its lighter homologues zinc and cadmium. (2) Work on the search of global and local minima of gold-palladium clusters important for catalytic processes. (3) Strengthening existing research collaborations with F. Calvo (France) and M. Wormit (Germany), project (1)(c); and establishing the newly developed collaboration with M. Ehara (Japan) and N. Gaston (Victoria U), project (2). (4) Disseminate research results by publication in high-impact journals and conferences like e.g. the Wagga-Wagga conference (Waiheke, February, invited speaker), CMMSE 2014 (Spain, July, invited speaker).
- P. Schwerdtfeger will compete for a Marsden grant and continues to develop the Fullerene program suite together with James Avery and Lukas Wirz. He will also collaborate intensively with V. V. Flambaum on the search for the electron electric dipole moment. Further, new research will focus on nucleation of rare gas clusters using mathematical models (graph theory, kissing spheres for real systems) to solve a longstanding problem on phase transitions in cluster growth. For 2014, he is also an invited/plenary speaker at a number of international conferences overseas and organizer of two conferences (Spain and Germany). One PhD student (Mustafa Hasanbulli) will finish his thesis in 2014, and we expect a new postdoctoral fellow to arrive in March 2014 to work on joint projects with V. V. Flambaum. He will also take up more teaching for the chemistry major in 2014 (teaching environmental chemistry, geochemistry, chemical evolution theory, and introduction to quantum theory for chemists).

Appendix 2

1. Research Output, Publications and Reports

Articles published in 2013 refereed journals (members of CTCP are in bold letters):

1. I. V. Barashenkov, G. S. Jackson, **S. Flach**, “Blow up regimes in the PT symmetric coupler and the actively coupled dimer”, *Phys. Rev. A* **88**, 053817–1–8 (2013).
2. N. Bender, S. Factor, **J.D. Bodyfelt**, H. Ramezani, D.N. Christodoulides, F.M. Ellis, T. Kottos, “Observation of Asymmetric Transport in Structures with Active Nonlinearities”, *Phys. Rev. Lett.* **110**, 234101 (2013).
3. **J.D. Bodyfelt**, M.C. Zheng, R. Fleischmann, T. Kottos, “Scaling Theory of Heat Transport in Quasi-1D Disordered Harmonic Chains”, *Phys. Rev. E* **87**, 020101(R) (2013).
4. **A. Borschevsky**, M. Ilias, V. A. Dzuba, V. V. Flambaum, **P. Schwerdtfeger**, “Relativistic study of the nuclear-anapole-moment effects in diatomic molecules”, *Phys. Rev. A* **88**, 022125–1–6 (2013).
5. **M. Cadatal-Raduban**, T. Shimizua, K. Yamanoi, K. Takeda, M. H. Pham, T. Nakazato, N. Sarukura, N. Kawaguchi, K. Fukuda, T. Suyama, T. Yanagida, Y. Yokota, A. Yoshikawa, “Micro-pulling down method-grown $\text{Er}_3^+:\text{LiCaAlF}_6$ as prospective vacuum ultraviolet laser material”, *J. Cryst. Growth* **362**, 167–169 (2013).
6. F. Calvo, **E. Pahl**, **M. Wormit**, **P. Schwerdtfeger**, “Evidence for low temperature melting of mercury owing to relativity”, *Angew. Chem. Int. Ed.* **52**, 7583–7585 (2013); *Angew. Chem.* **125**, 7731–7734 (2013).
7. **A. Cetoli**, **J. Brand**, R. G. Scott, F. Dalfovo, L. P. Pitaevskii, “Snake instability of dark solitons in fermionic superfluids”, *Phys. Rev. A* **88**, 043639–1–8 (2013).
8. R. Devendra, N. R. Edmonds, **T. Söhnle**, “Computational and experimental investigations of the urethane formation mechanism in the presence of organotin(IV) carboxylate catalysts”, *J. Mol. Cat. A* **366**, 126–139 (2013).
9. G. Gligoric, **K. Rayanov**, **S. Flach**, “Make slow fast - how to speed up interacting disordered matter”, *Europhys. Lett.* **101**, 10011 (2013).
10. P. R. McGill, J. M. R. Muir, H. Idriss, **T. Söhnle**, “Formamide adsorption over the TiO_2 (110) surface: a theoretical study”, *RSC Advances* **3**, 16829–16839 (2013).
11. D. A. Götz, R. Schäfer, **P. Schwerdtfeger**, “The performance of density functional and wavefunction based methods for the 2D and 3D structures of Au_{10} ”, *J. Comput. Chem.* **34**, 1975–1981 (2013).
12. S. Gohr, S. Grimme, **T. Söhnle**, B. Paulus, **P. Schwerdtfeger**, “Pressure dependent stability and structure of carbon dioxide - a density functional study including long-range corrections”, *J. Chem. Phys.* **139**, 174501–1–8 (2013).
13. T. Hangele, M. Dolg, **P. Schwerdtfeger**, “Relativistic Energy-Consistent Pseudopotentials for Superheavy Elements 119 and 120 Including Quantum Electrodynamical Effects”, *J. Chem. Phys.* **138**, 174113–1–8 (2013).
14. N. Hansen, **J. R. Allison**, F. H. Hodel, W. F. van Gunsteren, “Relative Free Enthalpies for Point Mutations in Two Proteins with Highly Similar Sequences but Different Folds”, *Biochemistry* **52**, 4962–4970 (2013).
15. **M. Hasanbulla**, S. P. Rogovchenko, Y. V. Rogovchenko, “Dynamics of a Single Species in a Fluctuating Environment under Periodic Yield Harvesting,” *J. Appl. Math.* 167671–1–12 (2013).
16. T. V. Lapyteva, **J. D. Bodyfelt**, **S. Flach**, “Do nonlinear waves in random media follow nonlinear diffusion equations?”, *Physica D* **256–257**, 1–6 (2013).

17. **M. Lein**, J. A. Harrison, A. J. Nielson, "Identification of non-classical C-H...M interactions in early and late transition metal complexes containing the CH(ArO)₃ ligand", *Dalton Trans.* **42**, 10939–10951 (2013).
18. D. Leykam, **S. Flach**, O. Bahat-Treidel, A. Desyatnikov, "Flat band states: disorder and nonlinearity", *Phys. Rev. B* **88**, 224203–1–6 (2013).
19. M. M. Müller, **J. R. Allison**, N. Hongdilokkul, L. Gaillon, P. Kast, W. F. van Gunsteren, D. Hilvert, "Directed Evolution of a Model Primordial Enzyme Provides Insights into the Development of the Genetic Code", *PLOS Genetics* **9**, e1003187–1–9 (2013).
20. B. Opanchuk, R. Polkinghorne, **O. Fialko**, **J. Brand**, P. D. Drummond, "Quantum simulation of the early universe", *Ann. Phys. (Berlin)* **525**, 866–876 (2013).
21. B. Ostojić, P. Jensen, **P. Schwerdtfeger**, P. R. Bunker, "The predicted spectrum and singlet-triplet interaction of the hypermetallic molecule SrOSr", *J. Phys. Chem. A* **117**, 9370–9379 (2013).
22. **K. Rayanov**, G. Radons, **S. Flach**, "Decohering localized waves", *Phys. Rev. E* **88**, 012901–1–6 (2013).
23. S. Riedel, **P. Schwerdtfeger**, "Cesium Chemistry - Beyond State 1", *Nature Chem.* **5**, 815–816 (2013).
24. S. Rothe, A. N. Andreyev, S. Antalic, **A. Borschevsky**, L. Capponi, T. E. Cocolios, H. De Witte, E. Eliav, D. V. Fedorov, V. N. Fedosseev, D. A. Fink, S. Fritzsche, L. Ghys, M. Huyse, N. Imai, U. Kaldor, Y. Kudryavtsev, U. Köster, J. F. W. Lane, J. Lassen, V. Liberati, K. M. Lynch, B. A. Marsh, K. Nishio, D. Pauwels, V. Pershina, L. Popescu, T. J. Procter, D. Radulov, S. Raeder, M. M. Rajabali, E. Rapisarda, R. E. Rossel, K. Sandhu, M. D. Seliverstov, A. M. Sjödin, P. Van den Bergh, P. Van Duppen, M. Venhart, Y. Wakabayashi, K. D. A. Wendt, "Measurement of the first ionization potential of astatine by laser ionization spectroscopy", *Nature Commun.* **4**, 1835–1–6 (2013).
25. **P. Schwerdtfeger**, "One flerovium atom at a time", *Nature Chem.* **5**, 636 (2013).
26. **P. Schwerdtfeger**, **L. Wirz**, **J. Avery**, "Program Fullerene - A Software Package for Constructing and Analyzing Structures of Regular Fullerenes", *J. Comput. Chem.* **34**, 1508–1526 (2013).
27. W. Sheng, M. Wang, **M. Lein**, L. Jiang, W. Wei, J. Wang, "Mechanism of copper(I)-catalyzed allylic alkylation of phosphorothioate esters: influence of the leaving group on α regioselectivity", *Chem. Europ. J.* **19**, 14126–14142 (2013).
28. Y. Shinzato, K. Yamanoi, R. Nishi, K. Takeda, T. Nakazato, T. Shimizu, N. Sarukura, **M. Cadatal-Raduban**, K. Fukuda, S. Kurosawa, Y. Yokota, A. Yoshikawa, T. Togashi, M. Nagasono, T. Ishikawa, "Vacuum Ultraviolet Fluorescence Spectroscopy of Nd³⁺:LaF₃ Using Femtosecond Extreme Ultraviolet Free Electron Laser", *Appl. Phys. Express* **6**, 022401–1–4 (2013).
29. C. Skokos, I. Gkolias, **S. Flach**, "Nonequilibrium chaos of disordered nonlinear waves", *Phys. Rev. Lett.* **111**, 064101–1–5 (2013).
30. K. Smith, T. Carroll, **J.D. Bodyfelt**, I. Vitebskiy, and A.A. Chabanov, "Enhanced Transmission and Giant Faraday Effect in Magnetic Metal-Dielectric Photonic Structures", *J. of Phys. D: Appl. Phys.* **46**, 165002–1–5 (2013).
31. L. J. Smith, Y. Roby, **J. R. Allison**, W. F. Van Gunsteren, "Molecular dynamics simulations of barley and maize lipid transfer proteins show different ligand binding preferences in agreement with experimental data", *Biochemistry* **52**, 5029–5038 (2013).
32. L. J. Smith, W. F. Van Gunsteren, **J. R. Allison**, "Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12", *Protein Science* **22**, 56–64 (2013).
33. S.-W. Su, S.-C. Guo, A. Bradley, **O. Fialko**, **J. Brand**, "Kibble-Zurek Scaling and its Breakdown for Spontaneous Generation of Josephson Vortices in Bose-Einstein Condensates", *Phys. Rev. Lett.* **110**, 215302–1–5 (2013).

34. E. C. Y. Tam, L. M. Harris, E. S. Borren, J. D. Smith, **M. Lein**, M. P. Coles, J. R. Fulton, “Why compete when you can share? Competitive reactivity of germanium and phosphorus with selenium”, *Chem. Commun.* **49**, 10278–10280 (2013).
35. M. Tsuboi, K. Takeda, T. Nakazato, M. Kono, K. Yamanoi, **M. Cadatal-Raduban**, K. Sakai, R. Nishi, Y. Minami, M. V. Luong, Y. Arikawa, T. Shimizu, N. Sarukurua, T. Norimatsu, M. Nakai, H. Azechi, T. Murata, S. Fujino, H. Yoshida, A. Yoshikawa, N. Sato, H. Kan, K. Kamata “Electronic states of trivalent praseodymium ion doped in $20\text{Al}(\text{PO}_3)_3\text{--}80\text{LiF}$ glass”, *Jpn. J. Appl. Phys.* **52**, 062402–1–4 (2013).
36. **J. Wiebke**, **E. Pahl**, **P. Schwerdtfeger**, “Melting at High Pressure: Can First-Principles Computational Chemistry Challenge Diamond-Anvil Cell Experiments?”, *Angew. Chem. Int. Ed.* **52**, 13202–13205 (2013); *Angew. Chem.* **125**, 13442–13446 (2013).
37. **J. Wiebke**, **F. Senn**, **E. Pahl**, **P. Schwerdtfeger**, “Ab Initio Joule-Thomson Inversion Data for Argon”, *J. Chem. Phys.* **138**, 071105–1–3(C) (2013).
38. **J. Wiebke**, “Comment on ‘An equation of state for gaseous argon determined from the speed of sound’”, *Chem. Phys.* **411**, 43–44 (2013).
39. K. Yamanoi, T. Shimizu, **M. Cadatal-Raduban**, R. Nishi, K. Takeda, Y. Shinzato, T. Nakazato, N. Sarukura, T. Fukuda, M. Nagasono, T. Togashi, T. Satoh, T. Ishikawa, “Time-resolved pump and probe experiment for wide-gap semiconductors using free electron laser and synchronously-operated femtosecond laser”, *Jpn. J. Appl. Phys.* **52**, 040203–1–4 (2013).
40. K. Yamanoi, T. Murata, Y. Arikawa, T. Nakazato, **M. Cadatal-Raduban**, T. Shimizu, N. Sarukura, M. Nakai, T. Norimatsu, H. Nishimuraa, H. Azechi, S. Fujino, H. Yoshida, A. Yoshikawa, N. Satoh, H. Kan, “Luminescence properties of Nd^{3+} and Er^{3+} doped glasses in the VUV region”, *Opt. Materials* **35**, 1962–1964 (2013).
41. **X. Yu**, M. Müller, “Localization of disordered bosons and magnets in random fields”, *Ann. Phys.* **337**, 55–93 (2013).

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42. **O. Fialko**, **J. Brand**, U. Zuelicke, “Fragility of the fractional quantum spin Hall effect in quantum gases”, arXiv:1310.7283 [cond-mat.quant-gas] (2013).
43. E. Gerlach, S. Eggl, Ch. Skokos, **J.D. Bodyfelt**, G. Papamikos, “High Order Three Part Split Symplectic Integration Schemes”, *Proc. 10th HSTAM Intl. Congress on Mechanics*, arXiv:1306.0627v1 [nonlin.CD] (2013).
44. T. Kottos, N. Bender, S. Factor, **J. Bodyfelt**, H. Ramezani, D.N. Christodoulides, F.M. Ellis, “Taming the Flow of Light via Parity-Time Symmetry”, *Photonics Society Summer Topical Meeting Series, IEEE 2013*, 191–192 (2013).
45. **P. Schwerdtfeger**, **S. Biering**, **M. Hasanbulli**, **A. Hermann**, **J. Wiebke**, **M. Wormit**, **E. Pahl**, “High-Pressure Simulations – Squeezing the Hell out of Atoms”, *Proceedings of the 2012 International Conference on Computational and Mathematical Methods in Science and Engineering*, J. Vigo-Aguiar (Editor), Vol. 4, 2012; pgs. 1532–1533. Available at <http://gsii.usal.es/~CMMSE/images/stories/congreso/4-cmmse-2012.pdf>, ISBN 978-84-615-5392-1. (not listed in the 2012 report)

Chapters in Books:

none

General Scientific Writing:

none

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](http://ctcp.massey.ac.nz/index.php?group=&page=fullerenes&menu=fullerenes)

*Picture left (designed by J. Avery): T-C₃₈₀,
the first fullerene that does not admit any
face spirals, partially assembled until the
point where the spiral fails. Below the
fullerene a schematic drawing of the
partially spiralled fullerene graph is shown.
The T-C₃₈₀ molecule was generated with
program Fullerene using a generalized
spiral algorithm. Program Fullerene an
open-source code freely available at
Massey University's web-site and used by
many research groups world-wide. T
appear as cover picture in J. Chem. Inf.
Model.*

2. Conference and Workshop Presentations

Lectures at Conferences / Meetings:

- J. Allison was an invited speaker at the CECAM workshop on "Intrinsically Disordered Proteins: Connecting Computation, Physics and Biology" in Zürich, Switzerland, 2-5 September 2013, where she spoke on the topic "*Can simulations rationalise differing aggregation propensities of related disordered proteins?*"; the E3: Enzyme Engineering and Evolution meeting in Queenstown, New Zealand, 25-26 August 2013, where she spoke about "*Alice in molecular-land: an evolutionary arms race in sequence and structure space*"; and the Retirement Symposium of Prof. Wilfred van Gunsteren held at ETH Zürich, Switzerland, 16 May 2013, where her talk was entitled "*Back to the future: lysozyme revisited*".
- J.D. Bodyfelt gave a contributed talk entitled *Detangling Flat Band Lattices Via Fano Structures* at the Dodd-Walls 7th Annual Symposium in Dunedin on Nov. 12th, 2013.
- J. Brand gave invited talks at the conferences FINES-2013: Finite-Temperature Non-Equilibrium Superfluid Systems in Queenstown 16-20 February 2013; 3rd international conference: Nonlinear Waves – Theory and Applications in Beijing, 12-15 June 2013; 7th Cross-Strait and International Conference on Quantum Manipulation in Beijing, 28-30 June 2013; 22nd International Laser Physics Workshop in Prague, 15-19 July 2013; and the 7th Annual Dodd-Walls Symposium in Dunedin 12 November 2013.

- Carlo Danieli gave a contributed talk on *Approximating Metal-Insulator Transition* at the Dodd-Walls Meeting in Dunedin, 11-13 November, 2013.
- S. Flach gave invited talks at the IV international Symposium on Strong Nonlinear Vibronic and Electronic Interactions in Solids, Tartu, May 1-3, 2013; at The Third International Conference: Nonlinear Waves--Theory and Applications Beijing, June 12-15, 2013; at the workshop Methods of Chaos Detection and Predictability: Theory and Applications 17 - 21 June 2013, Dresden, Germany (and 1 week stay as guest scientist at MIPKs Dresden); at the International Conference on Phononics and Thermal Energy Science 1-4 September 2013, Shanghai, China; at the workshop Advances in Quantum Chaotic Scattering: From (Non-)Linear Waves to Few-Body Systems, 9-13 September 2013, Dresden Germany; at the workshop Lattice Differential Equations, 15-21 September 2013 Oberwolfach Germany; at symposium 20 years MIPKs Dresden, 11.11.13 - 15.11.13.
- E. Pahl gave invited lectures on *Melting of weakly-bound nanoclusters: Monte Carlo simulations of mercury and rare gases under high pressure* at the AMN6 conference in Auckland (February 11-15), on *Influence of Relativistic Effects on the Melting of Mercury Hg* at the APCTCC conference in Gyeongju (Korea), July 10-13, and at the NZIC conference (New Zealand Institute of Chemistry) in Wellington, December 1-5, on *Mercury's Low Melting Point: Influence of Relativistic Effects*.
- K. Rayanov gave a talks on "Amplification of evanescent waves - novel dynamical regimes with exciton-polariton condensates and optical couplers" at the "Advanced Workshop on Non-equilibrium Bosons: From Driven Condensates to Non-Linear Optics" in Trieste, Italy (August 20) and on "Amplification of evanescent waves - novel dynamical regimes with exciton-polariton condensates and optical couplers" at the "INMS Postgraduate Conference" in Auckland, New Zealand (October 23).
- P. Schwerdtfeger gave an invited lecture on *Playing with pentagons and heptagons – From fullerenes to carbon nanotubes and graphene* at the AMN6 conference in Auckland (February 11-15); a keynote lecture on *Playing with pentagons and heptagons – From fullerenes to carbon nanotubes and graphene* at the workshop on *Modern Methods in Quantum Chemistry*, Mariapfarr (Austria) 24.2-1.3; a keynote lecture on *Playing with pentagons and hexagons – The topology of fullerenes* at the WCAM2013 conference in Shanghai (June 5-7); an invited talk on *The Search for Electroweak Interactions in Chiral Molecules* at the *Spectroscopy of Fundamental Physics* Conference (June 17-21) at Columbus (Ohio); keynote lecture on *The topology of fullerenes* at the APCTCC conference in Gyeongju (Korea), July 10-13; invited talk on *Variation of Fundamental Constants in Space-Time* at the *Symmetry in Physics* conference, Bregenz, July 21-26; invited talk on *Quantum Electrodynamical Effects in Superheavy Elements* at the SHE (superheavy element) workshop in Takayama (Japan); September 19-21; invited lecture at the NZIC conference (New Zealand Institute of Chemistry) on *The topology of fullerenes*, Wellington, December 1-5.
- Xiaoquan Yu gave an invited talk on *Localization of disordered bosons and magnets in random fields* at the *Advanced Workshop on Non-equilibrium Bosons* (19-23 August) at The Abdus Salam International Centre for Theoretical Physics, Trieste (Italy); and an invited talk on *Nonlinear waves in disordered lattices with broken time reversal symmetry* at *2013 The Dodd-Walls Centre Symposium*, University of Otago (11-13 November).

Seminars and Talks:

- J. Brand gave invited seminar talks at ANU “From Josephson vortices to simulations of the universe with coupled Bose-Einstein condensates” (7 June 2013); at Peking University’s International Center for Quantum Matter (19 June 2013); and at Fujian Normal University (21 June 2013).
- S. Flach gave a lecture course (2 lectures) at the Theoretical Physics conference in Lille 21-25 January 2013; a Lecture Course (3 lectures) at the XIth Winter School on Theoretical Physics: Nanostructures and Nano-Scale Phenomena, Dubna, Russia, Jan 28 - Feb 3 2013; an invited seminar talk at the ANU Canberra 26.2.13 - 1.3.13; an invited colloquium at the physics department, University of Otago, 21 October 2013; an invited seminar talk at the ANU Canberra 15.12.13 - 18.12.13; an invited seminar talk at math department, University of Auckland, 24 October 2013.
- E. Pahl gave a lecture on *Melting of Mercury and Rare Gases* at a research meeting on clusters at the University of Christchurch, Cass Research Station, 30/10 – 1/11.
- P. Schwerdtfeger gave a GdCH lecture at Cologne University on “*Left or right in nature – The origin of biomolecular homochirality*” (May 28). Next day he gave a talk on *The topology of fullerenes* in the theoretical chemistry group at Cologne University; a seminar series on *Relativistic Pseudopotential Theory*, *High Pressure Physics* and on *Fullerenes* at the University of Napoli (June 25-29); a talk on the *Topology of Fullerenes* at the University of Milano (July 4).

Poster Presentations:

- Carlo Danieli presented a poster on *Approximating Metal-Insulator Transition* at the Advanced Workshop in Non- Equilibrium Bosons in Trieste, 19-23 August 2013.
- A. Muñoz Mateo and J. Brand presented a poster on *Three-dimensional solitary waves in confined BECs*, at the *7th Annual Dodd-Walls Symposium* in Dunedin, 11-13 November 2013.
- K. Rayanov presented a poster on "Actively coupled optical wave guides" at the "7th annual Dodd-Walls Symposium" in Dunedin, New Zealand (November 11).
- L. Wirz presented a poster on "Program Fullerene" at the AMN6 in Auckland, New Zealand (February 2013), and a poster on "Fullerene -- A Software Package for Constructing and Analysing Regular Fullerenes" at the APCTCC6 in Gyeongju, South Korea (July 11th, 2013).
- M. Hasanbuli presented a poster on “Confined Atomic Systems” at the AMN6 in Auckland, New Zealand (February 2013).

Appendix 3

1. RESEARCH

Current Areas of Research Activities:

Biomolecular Simulations
Cayley-Dickson Interpretations of Physics
Cluster Simulations and Phase Transitions, Nanoscience
Confined Atoms and Molecules
Development of new methods for electronic structure calculations
Electron Electric Dipole Moment
Electroweak Electronic Structure Theory
Frequency shifts in atomic clocks
Graph theoretical and topological properties of fullerenes
Heterogeneous and Homogeneous Catalysis
High-Pressure Physics
Integrated Nanophotonics
Macroscopic quantum superpositions
Nonlinear waves in Bose-Einstein Condensates
Nonlinear classical and quantum waves in disordered potentials
Non-equilibrium phase transitions
Non-perturbative QED
Nuclear anapole moment
One-dimensional quantum fluids
Password encryption with nonlinear waves at phase transitions
Parity-Time (PT) Symmetry in Distributed Gain-Loss Systems
Polariton condensate network dynamics
Parity violation in molecules
Quantum Chromodynamics
Quantum dynamics of ultra-cold few-atom systems
Quantum enhanced precision measurement
Quantum ratchets with ultracold atomic gases
Relativistic Quantum Chemistry
Single Parameter Scaling Theory of Disordered Systems
Solid State Physics
Spin-dependent parity violation in diatomic molecules
Stochastic Resonance
Strongly-correlated fermionic superfluids
Superheavy Element Chemistry
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
Tuneable Limit Cycles in Noisy Photonic Clocks
Variation of Fundamental Constants in Space-Time

2. PROFESSIONAL LEADERSHIP AND ADMINISTRATION

Honours and Awards:

- Elke Pahl received the 2013 Massey University Women's Award for her outstanding work on the accurate simulation of melting processes gaining international publicity (see picture below).
- Jane Allison received the 2013 INMS Research Award for her research progress in the past year.

Publicity:

- S. Flach updated the NZIAS web site.
- E. Pahl and P. Schwerdtfeger received world-wide publicity because of their paper on the low melting point of mercury, which featured in newspapers (mainly in Germany), news articles in Scientific American, Nature Chemistry and the New Scientist, cover page of Angewandte Chemie, and many more (see below). Our work also featured in the famous Periodic Table of Videos by produced by Brady Haran, a former BBC video journalist, featuring professor Martyn Poliakoff ("The Professor") (University of Nottingham, see <http://www.youtube.com/watch?v=NtnsHtYYKf0> with over 101,750 hits to this date).

Relativity behind liquidity

Mercury's low boiling point explained

Why mercury is a liquid at room temperature is a question that has puzzled scientists for over a century. Now, a team of researchers from Heidelberg University and the University of Mainz have found the answer. The team, led by physicist Dr. Michael Wormit, has shown that the low boiling point of mercury is due to the relativistic effects of the electrons in the atoms. This discovery could have implications for the development of new materials and the understanding of the behavior of other elements.

03.09.13 PHYSIK

Warum Quecksilber bei Raumtemperatur flüssig ist

Heidelberger Wissenschaftler haben mit einer Computersimulation herausgefunden, dass das Metall Quecksilber erst bei 120 Grad Celsius schmelzen würde – wenn es nicht die Relativitätstheorie gäbe.

NATURE CHEMISTRY | RESEARCH HIGHLIGHTS

ELEMENTAL MERCURY
State oddity

Anne Pichon

Nature Chemistry 5, 640 (2013) doi:10.1038/nchem.1722
Published online 23 July 2013

DIE WELT

03.09.13 | Physik

Warum Quecksilber bei Raumtemperatur flüssig ist

Heidelberger Wissenschaftler haben mit einer Computersimulation herausgefunden, dass das Metall Quecksilber erst bei 120 Grad Celsius schmelzen würde – wenn es nicht die Relativitätstheorie gäbe. Von Norbert Lossau

SCIENTIFIC AMERICAN

Permanent Address: <http://blogs.scientificamerican.com/the-curious-wavefunction/2013/07/31/what-does-mercury-being-liquid-at-room-temperature-have-to-do-with-einsteins-theory-of-relativity/>

By Ashish Jogalekar | July 31, 2013

What does mercury being liquid at room temperature have to do with Einstein's theory of relativity?

One of the great moments in twentieth century science came when Paul Dirac married quantum mechanics with Einstein's Special Theory of Relativity to produce relativistic quantum mechanics. Dirac's theory did many things – predict electron spin and the positron, analyze atomic collisions, jump-start the revolution in quantum electrodynamics – but it also had very significant repercussions for chemistry. However these repercussions did not become known for another few decades because it turned out that for solving most problems in chemistry you could neglect relativistic effects. Figuring out chemical bonding, predicting the thermodynamic properties of molecules and rates of chemical reactions, understanding the molecular glue that holds proteins together; all these problems succumbed to calculation without chemists worrying about relativity.

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WEITERE INFORMATIONEN

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Arbeitsgruppe Theoretische Chemie
Prof. Dr. Andreas Dreuw

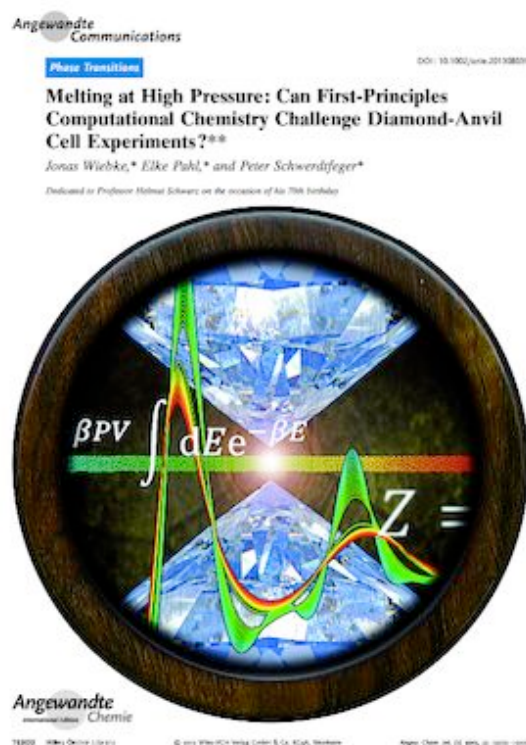
Albert Einsteins spezielle Relativitätstheorie weist den Weg zur Lösung des Geheimnisses des Quecksilbers

Das „Geheimnis“ des Quecksilbers hat ein internationales Forscherteam unter Beteiligung von Wissenschaftlern der Universität Heidelberg mit Hilfe von Computereperimenten gelöst. Auf der Basis von Simulationen und numerischen Verfahren sind sie der Frage nachgegangen, warum dieses Metall bei normalen Umgebungstemperaturen stets in flüssiger Form auftritt. Dabei konnten die Forscher aus Neuseeland, Frankreich und Heidelberg nachweisen, dass der niedrige Schmelzpunkt auf der besonderen Elektronenstruktur von Quecksilber beruht, die sich nur mit Hilfe der speziellen Relativitätstheorie (SRT) von Albert Einstein erklären lässt. Die Forschungsergebnisse wurden im Fachjournal „Angewandte Chemie“ veröffentlicht.

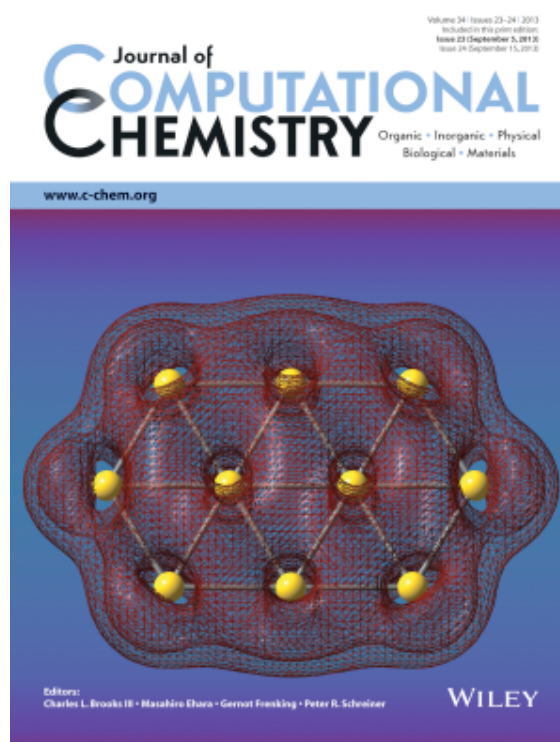
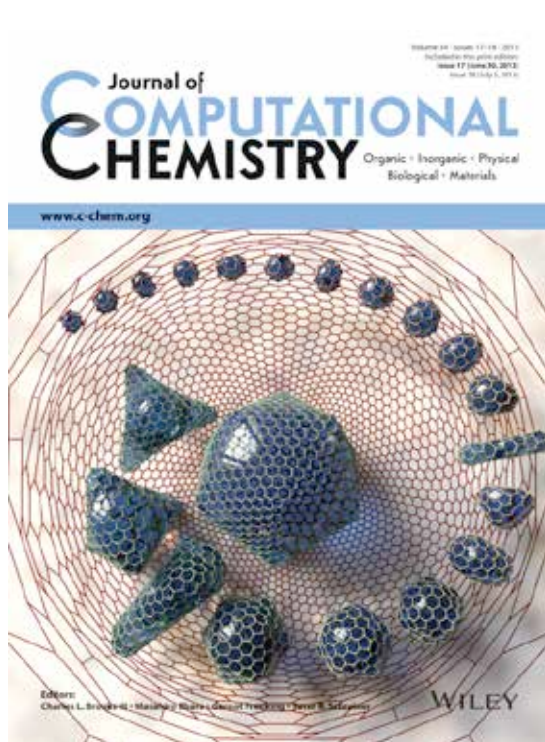
„Quecksilber stellt mit seinen Eigenschaften die theoretische Chemie seit langem vor viele Rätsel. Sein Aggregatzustand ist unter Normalbedingungen stets flüssig, anders als bei anderen Metallen wie Zink, Gold oder Kupfer, denen viel Wärme zugefügt werden muss, bis sie schmelzen“, sagt der Physiker Dr. Michael Wormit, der am Interdisziplinären Zentrum für Wissenschaftliches Rechnen (IWR) der Universität Heidelberg auf dem Gebiet der Theoretischen Chemie forscht. „Quecksilber ähnelt in seinem Verhalten häufig eher einem Edelgas als einem Metall.“

Das die Besonderheiten von Quecksilber bei Ursache in Effekten der speziellen Relativitätstheorie haben, wird in der

- E. Pahl, P. Schwerdtfeger and J. Wiebke had a cover page in *Angewandte Chemie* on high-pressure simulations challenging diamond-anvil cell experiments (see below).



- P. Schwerdtfeger had two cover pictures in *Journal of Computational Chemistry*: Program Fullerene – A Program to construct fullerenes and to perform a topological analysis (left, designed by the co-author J. Avery), and a paper on high precision calculations on the Au_{10} cluster (right). He was also interviewed by the German Newspaper Frankfurter Allgemeine on science policy in New Zealand.



Appendix 4

POST-GRADUATE SUPERVISION

Ongoing PhD Theses:

- Carlo Danieli (first year): *Many-body interactions in quasi-periodic potentials*, Supervisor: S. Flach.
- M. Hasanbulli (third year): *Atoms in Spherical Confinements*. Supervisors: P. Schwerdtfeger and B. Pavlov
- A. Punnett (fourth year): *How Hadrons keep their Quarks*. Supervisor: P. Bowman.
- Kristian Rayanov (first year): *Active coupling in optical couplers and exciton-polariton condensates*, Supervisor: S. Flach)
- Lukas Wirz (second year): *Computer Modelling of Fullerenes / Biasing molecular modelling with experimental RDCs*. Supervisors: P. Schwerdtfeger and J. Allison

Finished MSc Theses:

none

Teaching:

- J. Allison was involved in the fourth year paper *Research Methods in Molecular Biosciences* (162.760) and taught modules on: in-cell NMR spectroscopy, for the paper *Molecular Cell Biology* (122.704); DNA structure, for the paper *Genes and Gene Expression* (122.231); protein structure, for the paper *Biochemistry of Cells* (122.102); biochemical principles, for the paper *Chemistry for Biological Systems* (123.172) and the summer *Accelerated Program* (123.171/172); biochemistry and sustainability, for the paper *Science and Sustainability* (246.201); and biochemical modelling, for the paper *Systems and Models* (246.201), for which she is also the course coordinator and designer.
- J. D. Bodyfelt taught a thermodynamics module for the paper *Physics Ib* (124.102), and cooperated with S. Flach and J. Brand in writing/teaching five computer simulation laboratories (using Python's free interactive notebooks), for the paper *Nonlinear Physics & Chaos* (124.261).
- P. Bowman taught into the first year physics papers for scientists and engineers (124.101/171/102/172) -- including the August intake variant -- and the foundational BNatSci paper 246.102. He coordinated Astronomy (124.129) and the second year quantum and statistical mechanics paper (124.226).
- J. Brand is paper coordinator for and designed and taught (together with S. Flach and J. Bodyfelt) the new-in-2013 paper 124.261 *Nonlinear Physics and Chaos*. He also taught into 246.101 *Systems and Models* and 124.101 *Physics Ia*.
- S. Flach gave a second year course on *Nonlinear Physics and Chaos* (together with Joachim Brand) during second semester.
- E. Pahl is paper coordinator of 124.111 – *Physics for Life Sciences* and taught this paper (together with Marilou Catadal-Raduban) including lab teaching; gave a second year course on *Statistical Physics* within the 124.226 – *Quantum and Statistical Physics* paper and taught into the new accelerated 124.171/172 paper.
- P. Schwerdtfeger gave a lecture course on *Introduction to Computational Chemistry* within the paper *System and Models* for BNatSci 246.201 (semester 2) including hands-on computer simulations.

Other activities:

Papers refereed:

- J. Allison refereed papers for the journals PLoS One and J. Chem. Theory Comput. She is also a F1000 Associate Faculty Member, and refereed fellowship applications for the Engineering and Physical Sciences Research Council (EPSRC, UK), where she is a Peer Review College member.
- J. Bodyfelt refereed papers for Phys. Rev. A, Phys. Rev. E, and J. Phys A: Math. Theor.
- J. Brand refereed papers for New J. Phys., Phys. Rev. Lett., Phys. Rev. A, J. Phys. B. He also refereed grants for the European Science Foundation and the Israeli Science Foundation.
- A. Muñoz Mateo refereed papers for New J. Phys., and for Phys. Rev. A.
- P. Schwerdtfeger refereed in total 55 papers (rejecting about 2/3 of the invitations) from international journals including Angewandte Chem. Int. Ed., Chem. Phys. Chem., Chem. Phys. Lett., J. Am. Chem. Soc., J. Comput. Chem., J. Chem. Phys., J. Phys. Chem. A, J. Phys. Cond. Mat., Nature, Nature Chemistry, Phys. Chem. Chem. Phys., Phys. Rev. A, Phys. Rev. B, Phys. Rev. Lett., Theoret. Chem. Acc. and many more. He also was a referee for the grant agency Agence National de la Recherche (France).
- M. Catadal-Raduban refereed one paper for Optics Commun. and two papers for IEEE Trans. Nucl. Sci.

PhD/MSc and other theses refereed:

- J. Allison examined one B.Sc.Hons thesis and one PGDipSci thesis from the University of Auckland (Dec 2013).
- E. Pahl refereed and examined a PhD thesis from University of Wellington (Feb 2013)
- P. Schwerdtfeger refereed one PhD thesis from the University of Auckland, and one from the University of Otago. He also refereed a habilitation thesis from the University of Salzburg.

Conference Organisation:

- J. Allison is on the organisation committee for the Queenstown Molecular Biology meeting in August 2014.
- J. Brand organised a symposium on Quantum Degenerate Systems at the conference *Nonlinear Waves – Theory and Application* in Beijing 12-15 June 2013 and co-organised (with S. Flach) the NZIAS Symposium *Physics of Complex Systems*, Dec 20 2013 Albany.
- S. Flach was coordinator for the Advanced Workshop on *Non-Equilibrium Bosons: From Driven Condensates to Non-Linear Optics*, Aug 19-23 2013, ICTP, Trieste, Italy, ICTP fund: 25000 Euro; coordinator for the *International Workshop Nonlinear Dynamics at the Nanoscale*, Aug 25-30 2013 APCTP Pohang Korea, APCTP fund: 25000 Euro; coordinator for the NZIAS Symposium *Physics of Complex Systems*, Dec 20 2013 Albany.

Conference Participation:

- P. Schwerdtfeger participated at the Australian Humboldt meeting in Sydney, September 16-20, where he gave two short speeches and participated in a round-table discussion on science policies in Australia and New Zealand.

Chairs at Conferences:

- J. Brand chaired a session at the conferences 7th Cross-Strait and International Conference on Quantum Manipulation in Beijing, 28-30 June 2013; 22nd International Laser Physics Workshop in Prague, 15-19 July 2013; and the 7th Annual Dodd-Walls Symposium in Dunedin 12 November 2013.
- E. Pahl chaired a Physical Chemistry session at the NZIC conference in Wellington, December 1-5.

Boards / Editorial Boards / Professional Societies:

- P. Schwerdtfeger served on the editorial board for *Journal of Computational Chemistry*, *Wiley Interdisciplinary Reviews: Computational Molecular Science*, *Computational and Theoretical Chemistry* (Elsevier) and *The International Journal on Nanoelectronics and Materials*. He also served as the President of the New Zealand Humboldt Association (ending his term in 2013), and served on the board of the Asian-Pacific Association of Theoretical and Computational Chemists and on the International Academy of Quantum Molecular Science. Further he served as a member of the Academic Leadership team and of the INMS Exec Board at MU, which met July 6-7 in Menton (France).

Community Outreach:

- J. Allison gave seminars on her research at the Biology Olympiad selection camp and Rotary National Science and Technology Forum for secondary school students.
- P. Bowman gave talks to year 13 students at Orewa College.
- E. Pahl gave a course on *Striving for absolute zero*, for year 12 students within the STEM day at Massey University, Albany, July 2013. He also gave talks to high-school students at the Rotary Summer Science Camp
- P. Schwerdtfeger and Dr. Heather Hendrickson were part of a biology themed line-up that drew the largest attendance to date at this layperson gathering of science aficionados. Nerd nite (see picture right) is a fun evening, open to the public, where 3 short talks involving nerdy awesomeness are given at a bar in Kingsland.



Visits:

- J. Allison visited the research groups of Prof. Wilfred van Gunsteren (ETH Zurich) and Prof. Jonathan Essex (University of Southampton), Prof. Chris Dobson and Prof. Michele Vendruscolo (Cambridge University), and the researchers Lorna Smith (University of Oxford), Andrew Baldwin (University of Oxford), Sereina Riniker (ETH Zurich) and Janet Kumita (Cambridge University).
- E. Pahl visited the research group of Prof. Andreas Dreuw at the University of Heidelberg.
- P. Schwerdtfeger visited a number of universities in Europe for potential future research collaborations, including Napoli, Parma, Stuttgart, Darmstadt, Cologne and Marburg.

Appendix 4

Financial Statement:

Beside financial support from the College of Sciences through INS and NZIAS, which covers salaries and administrative support, the following income through internal and external grants was received in 2013 (in NZ\$):

Grants Received/Continuing:

- J. Brand, Marsden grant MAU0910 (final year)	21,158
- J. Brand, IVRF for visit of Nimrod Moiseyev (Feb. 2013)	3,350
- Oleksander Fialko (1 st year Marsden FastStart) on “Understanding quantum thermodynamics with the smallest heat engine”.	115,000
- Florian Senn, Swiss Science Foundation	33,000
- S. Flach, Distinguished Overseas Visitors Fund	10,000
- S. Flach, MURF Visitor funding	5,000
- E. Pahl (MU Women’s Award)	9,979
- P. Schwerdtfeger (US\$300 for talk at the Ohio State Univ.)	370

TOTAL	\$ 197,807
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Appendix 5

Staffing



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

Daniel Götz, Elke Pahl, Urban Rohrmann, Lukas 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: Joshua Bodyfelt, Thomas Ernst, Anastasia Borschevsky, Andreas Hauser, Michael Wormit, Mustafa Hasanbulli, Susan Biering, Ulrich Zülicke (Victoria University of Wellington), Gabriele Jaritz, and Tilo Söhnel.

Personnel:

Distinguished Prof. Peter Schwerdtfeger (Chemistry, Director of CTCP)
Prof. Joachim Brand (Physics, Deputy Director of CTCP)
Prof. Sergej Flach (Physics)
Dr. Jane Allison (Lecturer, Biological Sciences)
Dr. Joshua Bodyfelt (Research Officer)
Dr. Patrick Bowman (Senior Lecturer, Physics)
Dr. Elke Pahl (Lecturer, Physics)
Dr. Marilou Cadatal-Raduban (Senior Tutor, Physics)

Honorary CTCP Members:

Dr. Matthias Lein
Dr. Tilo Söhnel
Prof. Uli Zülicke

Secretaries:

Vesna Davidovic-Alexander (IAS)

Coleen van Es (INMS)

PhD Students:

Carlo Danieli (Supervisor: S. Flach)

Mustafa Hasanbulli (Supervisor: P. Schwerdtfeger)

Andrew Punnett (Supervisor: P. Bowman)

Kristian Rayanov (Supervisor: S. Flach)

Lukas Wirz (Supervisors: P. Schwerdtfeger and J. Allison)

MSc Students:

none

Exchange Students:

Daniel Götz, Darmstadt, PhD studies on gold and lead clusters

Research Assistant:

Sophie Shamilov (Supervisor: J. Brand)

Postdoctoral/Research Fellows:

Dr. Alberto Cetoli (Wenner-Gren Postdoctoral Fellow)

Dr. Oleksandr Fialko (Marsden fellow)

Dr. Antonio Munoz-Mateo (MU Postdoctoral Fellow)

Dr. Florian Senn (Swiss Science Foundation)

Dr. Jonas Wiebke (DAAD fellow)

Dr. Xiaoquan Yu (MU Postdoctoral Fellow)

Visitors from other institutions:*Long Term:*

Prof. Victor Flambaum (University of New South Wales, Australia) for 1 month, delivered two lectures on fundamental problems in physics and collaborated with P. Schwerdtfeger on nuclear anapole moments.

Prof. Phil R. Bunker (Canada) to collaborate on spectroscopic properties of heavy metal hyperoxides.

Prof. Tassos Bountis (Patras, Greece) for 2 months, delivered a 6 hour lecture course to CTCP/NZIAS/INMS members (approx 20 participants), an INMS seminar, discussion of possible research project with Carlo Laing. MURF: 2400\$ travel, NZIAS fund: 1600\$ locals

Prof. Igor Barashenkov and Dr. Nora Alexeeva (Cape Town, South Africa) for 5 months, worked with S. Flach and K. Rayanov on a joint project in optics, submitted one paper, another one is in preparation, delivered a CTCP/NZIAS/INMS seminar. NZIAS fund; 8000\$ locals, rest funding from UCT South Africa.

Prof. Masahiro Ehara (Institute for Molecular Science, Okazaki, Japan) 2 weeks visit to start a collaboration with E. Pahl on the structure of gold-palladium clusters.

Prof. Mark Hoffmann (University of Dakota, USA) for 2 months to collaborate on quantum electrodynamic effects in heavy atoms.

Peter Matthies and Alisa Podgurskaya (Moscow, Russia) for 1.5 months as exchange students, to work with Jane Allison (Matthies) and Tony Mutukumira (Podgurskaya). Fully funded by Moscow Institute of Physics and Technology.

Prof. Richard Mawhorter (Millikan Laboratory, USA) to collaborate on electric field gradients in diatomic molecules.

Prof. Nimrod Moiseyev (Technion, Israel) for four weeks.

Daniel Leykam (Canberra, Australia) for 11 days, will deliver a CTCP seminar, continue collaboration with S. Flach and initiate collaboration with Joshua Bodyfelt and Carlo Danieli. ANU Canberra fund: travel, NZIAS fund: 500\$ locals

Prof. Boris Altshuler (Columbia U, NY USA) 3 weeks visit.

Prof. Berny Schlegel (Wayne State University) 4 weeks visit to collaborate on relativistic effects in solvated gold complexes.

Dr. Ralf Tonner (Marburg University) for 1 month to collaborate on density functional calculations on large fullerene structures.

Short Term:

Prof. Blair Blakie (U Otago) symposium speaker.

Prof. Howard Carmichael (U Auckland) symposium speaker.

Dr. Anton Desyatnikov (Canberra, Australia) for 3 days, delivered a CTCP/NZIAS/INMS seminar, finalized and submitted one paper with S. Flach. Fully funded by ANU Canberra.

Dr. Nicola Gaston (U Victoria) seminar.

Prof. Mark S. Gordon (Iowa State University and Ames Laboratory, U.S.A.).

Prof. Michele Governale (U Victoria) symposium speaker.

Prof. Sarukura (Osaka University, Osaka, Japan).

Prof. Ronnie Kosloff (Hebrew University of Jerusalem), seminar speaker.

Prof. Gary B. Schuster (Georgia Institute of Technology, USA).

Prof. Pavlo Selyshchev (U Pretoria, SA), seminar speaker.

Prof. Yehuda Band (Ben Gurion University, Israel), seminar speaker.

Prof. Michael Fleischhauer (University of Kaiserslautern, Germany), seminar speaker.

Dr. Simon Gardiner (University of Durham, UK), seminar speaker.

Dr. Dario Poletti (SUTD Singapore), seminar speaker.

Prof. Thomas Gasenzer (University of Heidelberg, Germany), seminar speaker.

Prof. Sandro Wimberger (University of Heidelberg, Germany), seminar speaker.

Prof. Shih-Chuan Guo (Changhua University of Education, Taiwan), collaborator and seminar speaker.

Prof. Peter Drummond (Swinburne University of Technology, Australia), collaborator and seminar speaker.