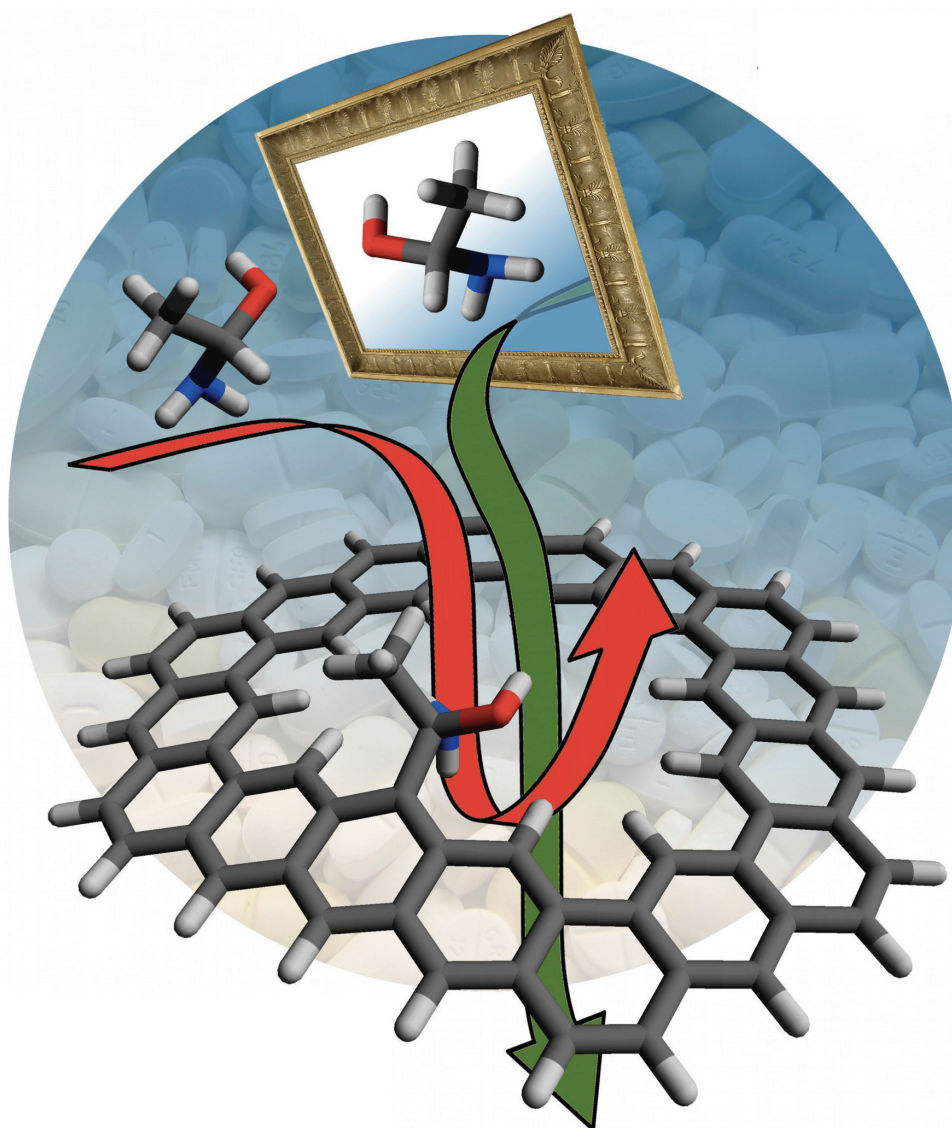


**CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)**  
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**INSTITUTE OF NATURAL AND MATHEMATICAL SCIENCES (INMS)**  
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**2014 MASSEY UNIVERSITY ANNUAL REPORT**  
**CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS**



**T**he attachment of a suitable “bouncer” molecule to the rim of a graphene pore prevents the passage of the undesired enantiomer while letting its mirror image through. A small difference in the geometry of the temporary dimer complex, which is formed by the “bouncer” and the penetrating molecule, is transformed into a significant difference for the transmission barrier.  
 (picture designed by Andreas Hauser).

**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 one of the most productive research centres here in New Zealand, with truly outstanding performances by each of our eight staff members. Our research centre has not been without a Marsden grant running since it was established (a new grant was awarded in 2014), three staff are actively involved in the newly formed Dodd-Walls CoRE, two staff have received research medals (Jane Allison the *MU Early Career Research Medal* and Peter Schwerdtfeger the *Rutherford Medal*), our articles appear regularly in top international journals such as *Physical Review Letters* or *Angewandte Chemie*. The many high-standing international visitors who joined our research centre in 2014, and the many invitations to international conferences received by our staff, are a clear indication of our success.

**Research Output:** This year we published 40 articles in journals and books.

**Activities and achievements:** All members of CTCP were involved in chemistry, physics or biology teaching as outlined in Appendix 4. Almost all postdoctoral fellows helped in laboratory teaching at year 1 level. All articles are published in highly acclaimed international journals of high impact factor. Our research centre received one new full Marsden grant this year (Elke Pahl and Peter Schwerdtfeger). Amongst the outstanding achievements were awards of two research medals. The large number of international eminent visitors we get each year clearly underlines our international visibility and high level of achievement.

**The Future - Opportunities, Risks and Directions:** We are a top research centre of international exceptional high standing. This we achieved despite the rather limited financial resources available to our research centre. The risks are very clear: Other universities overseas are far better resourced and the loss of excellent staff is inevitable. On the good news side is a grant of 180,000 NZ\$ to upgrade and maintain our CTCP compute cluster in 2015.

**Work in progress:** There are too many research projects in progress to list all of them (see attachment for more details). Funding in 2015 is anticipated mainly through Marsden Grants and the Dodd-Walls CoRE (see appendix 1). A 180,000\$ grant by Massey University College of Science has been approved to upgrade our current *Double-Helix Supercomputer* cluster. Upgrades have been purchased and consist of a 8,000\$ in cluster management/OS software, a new head node, 20 new compute nodes housed in 5 server chassis, two ethernet switches, and a complete FDR Infiniband network. In the start of 2015, the rats-nest behind the equipment racks in PABX (where the cluster is housed) will be cleanly re-cabled and labelled to accommodate the new build. The new head node and servers will be installed, and branded as *Simurg*. The current in-situ nodes, labelled *Marvin*, will then be taken offline and migrated into *Simurg*. Discussions with INMS will also continue – we propose to migrate INMS' *Zaphod* cluster as a *Simurg* queue. At completion, the older node registries of *Marvin/Zaphod* will be retired. In addition to the technical operations, public relations also commence: a new user wiki has been designed for *Simurg* (which can be viewed at <http://www.massey.ac.nz/~theochem/simurg>), and we look forward to making our official announcement of *Simurg* in Spring 2015.

**Staffing:** 2014 saw a number of additions to our research centre. Lukas Trombach, a new PhD student in the groups of Pahl and Schwerdtfeger, joined our centre in December this year. Jayson Cosme started his PhD jointly with J. Brand and O. Fialko. Sophie Shamilov started her PhD with J. Brand. And finally, Mustafa Hasanbulli (Supervisors: B. Pavlov and P. Schwerdtfeger) handed in his PhD thesis.

**Financial:** See Appendix 4.

**Acknowledgment:** The Director is grateful to all CTCP members for their (again) outstanding performance and very hard work in 2014, and wishes everybody an even more successful year 2015. 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).

A handwritten signature in black ink, appearing to read 'Peter Schwerdtfeger', with a stylized flourish at the end.

Distinguished 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 and Teaching Objectives for 2015

- J. R. Allison will continue the work funded by her 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 ETH Zurich. This is being carried out by her PhD students Elisey Kobzev, funded by a Commonwealth Scholarship, and Ivan Welsh, funded by the Marsden grant. Ivan will also continue his work on automated construction of atomic-level force field parameters as part of a collaborative project with the group of Prof. Alan Mark at the University of Queensland, in addition to his other projects on enhanced sampling methods (with Deborah Crittenden, University of Canterbury) and an exciting new Bayesian method for extracting structural information from neutron diffraction of disordered materials (with Prof. Andrew Goodwin, University of Oxford). A third PhD student, Ashar Malik, will work on using molecular dynamics (MD) simulations to increase the statistical robustness of the infant field of structural phylogenetics, which has the possibility to probe deep evolutionary relationships. This work is in collaboration with Assist. Prof. Anthony Poole (University of Canterbury); we aim to write a full Marsden application about this work in 2015. Having gained his MSc with Distinction, William Irvine has now begun a PhD funded by a Massey University Doctoral Scholarship. He will continue his work with Jack Flanagan at the Auckland Cancer Research Institute investigating the interaction of wild-type and oncogenic mutations of PI3K $\alpha$  and related kinases with the ultimate aim of developing new drugs. William will also work on a new project with Assist. Prof. Joel Tyndall (Otago University) looking at the binding and release of lipids by a membrane-bound cytochrome P450, and will submit for publication a manuscript describing the lipid parameters he developed during his MSc. Lukas Wirz, Jane's fifth PhD student, will submit his PhD thesis early in 2015. By then he will have submitted two further journal articles in addition to the one currently under review. Jane will look to publish her collaborative work on combining NMR data with MD simulations (with Lorna Smith, University of Oxford). She is also developing a new project designing peptides and small molecules to inhibit protein-protein interactions implicated in cancer with INMS staff member Evelyn Sattler, and is involved in potentially game changing research into the true reason for the temperature-dependence of enzyme activity with Prof. Vic Arcus (Waikato University). Finally, both of the non-Massey PhD students that Jane co-supervises (Davoud Zare, supervisor: Prof. Kate McGrath, Victoria University; Tatyana Pichugina, supervisor: Justin O'Sullivan, Liggins Institute), will submit their PhD theses in 2015, along with related publications.
- J. D. Bodyfelt: In 2014, I successfully built an internal business case to fund an \$180k upgrade to the Marvin computing cluster. Five server machines and a fiber optic network arrive in December, therefore my main objective for 2015 is to smoothly implement these within the running cluster, and update the cluster help website to a media-wiki format. In terms of fundraising, I will again attempt a Marsden application in order to support one PhD student and my conference travel. Also, I'd like to increase my research network to American colleagues, and perhaps look at eligible NSF funding or any AFOSR/ONR BAA opportunities. In terms of research topics, I shall: (a) continue fruitful collaborations with S. Flach on flat-band lattices in condensed matter, (b) finalize on-going studies of coupled semiconductor laser arrays with colleagues in Kazakhstan, and (c) finish two projects involving parity-time symmetry.



- P. Bowman is currently 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 occur in heavy atomic nuclei). Recently he started exploring the possibility of applying Lattice gauge techniques to problems in ultra-cold quantum gases with J. Brand.
- J. Brand will commence his role as Principal Investigator and Theme Leader for the Dodd-Walls Centre (DWC) of Research Excellence. Two DWC-funded postdocs will start on their projects on analogue quantum simulation of relativistic field theory with ultra-cold atoms and dynamics of spin-orbit coupled Bose gases, respectively. Joachim will also continue on research projects with Oleksandr Fialko (CTCP) and the group around Peter Drummond (Australia), where a paper on studying quantum decay of a false vacuum with ultra-cold atoms is about to be published. Other on-going research projects involve PhD student Sophie Shamilov looking at solitons in one-dimensional integrable quantum models and quantum dynamics in multi-configurational time-dependent Hartree for bosons (MCTDH-B) with PhD student Jayson Cosme. Joachim will further apply for Marsden funding for an emerging project with Max-Planck director Ali Alavi from Stuttgart/Cambridge on quantum Monte-Carlo calculations for ultra-cold atomic gases.
- S. Flach (Sergej) is working on a variety of research topics including quantum and classical many body localization, flatband physics, transport properties of novel optical waveguide networks, dissipative exciton-polariton condensate networks, symmetry analysis of ratchets, the impact of artificial gauge fields on ultracold atomic gases, among others. He strengthens his research collaboration with Yuri Kivshar's centre at ANU Canberra (Australia) which already resulted in three publications in Physical Review Letters, Europhysics Letters and Physical Review B. Together with Yuri Kivshar Sergej is part of a consortium running an Erasmus Mundus Exchange Program on Nanophotonics. Seven more European groups are part of that program, which is funded by the European Union with about 1.300.000 NZ\$. The program will run for four years and fund extended research visits of PhD students and postdoctoral fellows. Sergej is finalizing a project with Boris Altshuler at Columbia U NY (USA), whom he recently attracted for a long-term commitment as an external member of NZIAS at Massey University and a three-year funding through the Distinguished International Visitor Fund of Massey University. Sergej also attracted David Campbell at Boston U (USA) who was awarded with a one year Distinguished Visitor Fund of Massey University. Together with Joachim Brand he is coordinating the return Tandem workshop MIPKS-NZIAS in February 2015 in Rotorua. Further Sergej will coordinate a two-week workshop in the International Institute of Physics at Natal, Brazil in 2015. The successful series of NZIAS Christmas symposia will be continued with the third symposium in 2015 again. Sergej was recently appointed as director of the Center for Theoretical Physics of Complex Systems at the Institute for Basic Science in South Korea. His setting up of that center will open new opportunities of collaborations, research and exchange. Finally Sergej will deliver a number of invited talks, lectures and colloquia throughout the year at various top research centers and universities in Germany, USA, Ukraine, Italy, and other countries.
- E. Pahl will start work funded by the Marsden grant “Putting the squeeze on atoms and molecules: accurate quantum simulations of atomic and molecular phases under high pressures and temperatures” where she is co-PI together with P. Schwerdtfeger. First steps here are the recruitment and training of a new PhD student and a postdoctoral fellow who will start with in March (begin of the Marsden contract) or soon after. Another new PhD student, Lukas Trombach (co-supervised with P. Schwerdtfeger) just arrived mid of

December to work on solid-state behaviour and melting of nanoclusters and extended systems. Furthermore, she plans to intensify her successful collaboration with Prof. Masahiro Ehara from Japan on the structures of gold-palladium nanoclusters used in catalysis of organic reactions. In April she is invited to spend some weeks at the Institute of Molecular Sciences in Okazaka, Japan in the research group of Prof. Ehara. Continuation of work on the volume definition in Monte Carlo (MC) simulations of clusters in constant-pressure ensembles as well as on melting of molecular clusters ( $N_2$ ) is expected to lead to further research publications. This latter work will be supported by a month-long research visit of MC expert Dr F Calvo planned for the second half of the year. During that visit it is also planned to devise and write on a review on *Melting of Nanoclusters*. Several conference visits will be used to disseminate results of the research at international conferences including the AMN7 conference in Nelson in February and the ICQC conference in Beijing in June next year.

- Boris Pavlov will study of the alternation of the spectral modes and a beating phenomenon in an oscillator system with multiple eigen-frequencies under small perturbations. He will also work on a zero-range model of an active zone on a thin tectonic plate defined by an additional pressure and the relevant beating phenomenon for seismo-gravitational modes with close frequencies. H will further work on applications to an algorithm of earthquake prediction based on the monitoring of the beating phenomenon, and on modeling of the resonance interaction of the Bloch waves on multidimensional lattices, perturbed lattices and sandwiches.
- P. Schwerdtfeger will start on a Marsden grant together with Elke Pahl to simulate phase transitions and will continue to develop the Fullerene program suite together with James Avery and Lukas Wirz. He will also collaborate intensively with Victor V. Flambaum, Anastasia Borschevsky and Lukas Pasteka on the variation of fundamental constants in space-time. 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 2015, he is also an invited/plenary speaker at a number of international conferences overseas, organizer of a conference on the topology of fullerenes in Spain, organizer of several symposia within the Pacificchem conference in Hawaii (December 2015), and the Källen Lecturer for 2015 at the University of Lund. He will also attend the IAQMS meeting in Beijing to elect new fellows and will give a talk at the relativistic meeting at the same time in Beijing. One new PhD student (Lukas Trombach) will start on his thesis in 2015 working on cluster modeling, and we expect a new postdoctoral fellow to arrive in October 2015 to work on joint projects with E. Pahl. There are further commitments to deliver the Rutherford Lecture at various places in New Zealand. He will also contribute to teaching for the chemistry major in 2015 (environmental chemistry, geochemistry, chemical evolution theory, and introduction to quantum theory for chemists).

## Appendix 2

### 1. Research Output, Publications and Reports

Articles published in 2014 refereed journals (members of CTCP are in bold letters):

1. V. M. Adamyan, G. J. Martin, and **B. S. Pavlov**, “Local Inverse Scattering Problem as a Tool of Perturbation Analysis for Resonance Systems”, *Amer. Math. Soc. Transl.* **233**, 1-26 (2014).
2. N. V. Alexeeva, I. V. Barashenkov, K. Rayanov, **S. Flach**, “Actively coupled optical waveguides”, *Phys. Rev. A* **89**, 013848-1-5 (2014).
3. **J. R. Allison**, R. Rivers, J.C. Christodoulou, M. Vendruscolo, C.M. Dobson, “A relationship between the transient structure in the monomeric state and the aggregation propensities of  $\alpha$ -synuclein and  $\beta$ -synuclein”, *Biochem.* **53**, 7170-7183 (2014). (highlighted article and selected for cover)
4. **J. D. Bodyfelt**, D. Leykam, **C. Danieli**, **X. Yu**, **S. Flach**, “Flatbands under correlated perturbations”, *Phys. Rev. Lett.* **113**, 236403-1-5 (2014).
5. B. Boekfa, **E. Pahl**, N. Gaston, H. Sakurai, J. Limtrakul, M. Ehara, “C-Cl Bond Activation on Au/Pd Bimetallic Nanocatalysts Studied by Density Functional Theory and Genetic Algorithm Calculations”, *J. Phys. Chem. C* **118**, 22188-22196 (2014).
6. J. Cosme, **O. Fialko**, “Thermalization in closed quantum systems: Semiclassical approach”, *Phys. Rev. A* **90**, 053602-1-5 (2014).
7. S. Denisov, **S. Flach**, P. Haenggi, “Tunable transport with broken space-time symmetries”, *Phys. Rep.* **538**, 77-120 (2014).
8. **S. Flach**, D. Leykam, **J. D. Bodyfelt**, P. Matthies, A.S. Desyatnikov, “Detangling flat bands into Fano lattices”, *Europhys. Lett.* **105**, 30001-1-6 (2014); *Erratum* **106**, 19901 (2014). (selected as editor’s choice)
9. **O. Fialko**, “Decoherence via coupling to a finite quantum heat bath”, *J. Phys. B: At. Mol. Opt. Phys.* **47**, 045302-1-4 (2014).
10. **O. Fialko**, **J. Brand**, U. Zülicke, “Fragility of the fractional quantum spin Hall effect in quantum gases”, *New J. Phys.* **16**, 025006-1-17 (2014).
11. D. A. Götz, A. Shayeghi, R. L. Johnston, **P. Schwerdtfeger**, R. Schäfer, “Structures and dielectric properties of neutral lead clusters”, *J. Chem. Phys.* **140**, 164313-1-6 (2014).
12. R.S. Grand, T. Pichugina, L.R. Gehlen, M.B. Jones, P. Tsai, **J.R. Allison**, R. Martienssen, J.M. O’Sullivan. Chromosome conformation maps in fission yeast reveal cell cycle dependent sub nuclear structure. *Nucl. Acids Res.* **42**, 12585-12599 (2014) (breakthrough article and selected for cover)
13. S. Harder, D. Naglav, **P. Schwerdtfeger**, I. Nowik, Ro. H. Herber, “Metal Atom Dynamics in Superbulky Metallocenes: A Comparison of  $(\text{Cp}^{\text{BIG}})_2\text{Sn}$  and  $(\text{Cp}^{\text{BIG}})_2\text{Eu}$ ”, *Inorg. Chem.* **53**, 2188-2194 (2014).
14. A. W. Hauser, N. Mardirossian, J. A. Panetier, M. Head-Gordon, A. T. Bell, **P. Schwerdtfeger**, “Functionalized graphene as a gatekeeper for chiral molecules: A new concept for chiral separation”, *Angew. Chem. Int. Ed.* **53**, 9957-9960 (2014); *Angew. Chem.* **126**, 10117-10120 (2014). (awarded cover page)
15. A. Hermann, **P. Schwerdtfeger**, “Xenon sub-oxides stable under pressure”, *J. Phys. Chem. Lett.* **5**, 4336-4342 (2014).

16. M. V. Ivanchenko, T. V. Lapyteva, **S. Flach**, “Quantum chaotic subdiffusion in random potentials”, *Phys. Rev. B* **89**, 060301-1-4(R) (2014).
17. T. V. Lapyteva, M. V. Ivanchenko, **S. Flach**, “Nonlinear lattice waves in heterogeneous media”, Topical Review, *J. Phys. A* **47**, 493001-1-55 (2014).
18. R. Liao, Z. Huang, X. Lin, **O. Fialko**, “Spin-Orbit Coupled Bose Gases at Finite Temperatures”, *Phys. Rev. A* **89**, 063614-1-6 (2014)
19. A. Muñoz Mateo, **J. Brand**, “Chladni solitons and the onset of the snaking instability for dark solitons in confined superfluids”, *Phys. Rev. Lett.* **113**, 255302-1-5 (2014).
20. L. Morales-Molina, E. Doerner, **C. Danieli**, **S. Flach**, “Resonant extended states in driven quasiperiodic lattices: Aubry-Andre localization by design”, *Phys. Rev. A* **90**, 043630-1-5 (2014).
21. S. Nahrwold, R. Berger, **P. Schwerdtfeger**, “Parity violation in nuclear magnetic resonance frequencies of chiral tetrahedral tungsten complexes NWXYZ (X, Y, Z = H, F, Cl, Br or I)”, *J. Chem. Phys.* **140**, 024305-1-7 (2014).
22. T. Nakazato, T. Hori, T. Shimizu, K. Yamanoi, K. Sakai, K. Takeda, R. Nishi, Y. Minami, **M. Cadatal-Raduban**, N. Sarukura, H. Nishimura, H. Azechi, T. Fukuda, M. Tanaka, M. Nishikino, T. Kawachi, “Spatial Resolution Evaluation of ZnO Scintillator as an In-situ Imaging Device in EUV Region”, *IEEE Trans. Nucl. Sci.* **61**, 462-466(2014).
23. O. Ori, M. V. Putz, I. Gutman, **P. Schwerdtfeger**, “Generalized Stone-Wales Transformations for Fullerene Graphs Derived from Berge’s Switching Theorem”, *Math. Chem. Monographs* **16**, 259-272 (2014).
24. B. Ostojić, P. Jensen, **P. Schwerdtfeger**, P. R. Bunker, “Singlet-triplet interaction in Group 2 M<sub>2</sub>O hypermetallic oxides, *J. Mol. Spectr.* **301**, 20-24 (2014).
25. V. Pershina, **A. Borschevsky**, M. Ilias, “Theoretical predictions of properties and volatility of chlorides and oxychlorides of group-4 elements. I. Electronic structures and properties of MCl<sub>4</sub> and MOCl<sub>2</sub> (M = Ti, Zr, Hf, and Rf)”, *J. Chem. Phys.* **141**, 064314-1-8 (2014).
26. V. Pershina, **A. Borschevsky**, M. Ilias, A. Türlér, “Theoretical predictions of properties and volatility of chlorides and oxychlorides of group-4 elements. II. Adsorption of tetrachlorides and oxydichlorides of Zr, Hf, and Rf on neutral and modified surfaces, *J. Chem. Phys.* **141**, 064315-1-7 (2014).
27. M. H. Pham, **M. Cadatal-Raduban**, M. V. Luong, H. H. Le, K. Yamanoi, T. Nakazato, T. Shimizu, N. Sarukura, H. D. Nguyen, “Numerical simulation of ultraviolet picosecond Ce:LiCAF laser emission by optimized resonator transients”, *Jpn. J. Appl. Phys.* **53**, 062701-1-6 (2014),
28. U. Rohrmann, **P. Schwerdtfeger**, R. Schäfer, “Atomic domain magnetic nanoalloys - interplay between molecular structure and temperature dependent magnetic and dielectric properties in manganese doped tin clusters”, *Phys. Chem. Chem. Phys.* **16**, 23952-23966 (2014).
29. **F. Senn**, **J. Wiebke**, O. Schumann, S. Gohr, **P. Schwerdtfeger**, **E. Pahl**, “Melting of “non-magic” argon clusters and extrapolation to the bulk limit”, *J. Chem. Phys.* **140**, 044325-1-5 (2014).
30. T. Shimizu, K. Yamanoi, R. Arit, T. Hori, K. Fukuda, Y. Minami, **M. Cadatal-Raduban**, N. Sarukura, T. Fukuda, M. Nagasono, T. Ishikawa, “Optical property of Ce<sup>3+</sup>-doped lutetium lithium fluoride for the short-wavelength device application”, *Opt. Mat.* **36**, 1963-1965 (2014).



31. Ch. Skokos, E. Gerlach, **J. D. Bodyfelt**, G. Papamikos, S. Eggl, “High order three part split symplectic integrators: Efficient techniques for the long time simulation of the disordered discrete nonlinear Schroedinger equation”, *Phys. Lett. A* **378**, 1809-1815 (2014).
32. **J. Wiebke**, M. Wormit, R. Hellmann, E. Pahl, **P. Schwerdtfeger**, “Can an Ab-Initio Three-Body Virial Equation Describe the Mercury Gas Phase?” *J. Phys. Chem. B* **118**, 3392-3400 (2014).
33. **L. Wirz**, R. Tonner, J. Avery, **P. Schwerdtfeger**, “Structure and Properties of the Non-Spiral Fullerenes  $T\text{-C}_{380}$ ,  $D_3\text{-C}_{384}$ ,  $D_3\text{-C}_{440}$  and  $D_3\text{-C}_{672}$  and their Halma and Leapfrog Transforms”, *J. Chem. Inf. Mod.* **54**, 121-130 (2014). (awarded cover picture)
34. M. Wormit, M. Olejniczak, A.-L. Deppenmeier, A. Borschevsky, T. Saue, **P. Schwerdtfeger**, “Strong Enhancement of Parity Violation Effects in Chiral Uranium Compounds”, *Phys. Chem. Chem. Phys.* **16**, 17043-17051 (2014). (chosen as hot article by PCCP).
35. K. Yamanoi, R. Nishi, K. Takeda, Y. Shinzato, M. Tsuboi, M. V. Luong, T. Nakazato, T. Shimizu, N. Sarukura, **M. Cadatal-Raduban**, M. H. Pham, H. D. Nguyen, S. Kurosawa, Y. Yokota, A. Yoshikawa, T. Togashi, M. Nagasono, T. Ishikawa, “Perovskite fluoride crystals as light emitting materials in vacuum ultraviolet region”, *Opt. Mat.* **36**, 769-772 (2014).
36. **X. Yu**, **S. Flach**, “Enhancement of chaotic subdiffusion in disordered ladders with synthetic gauge fields”, *Phys. Rev. E* **90**, 032910-1-7 (2014).

### Refereed Conference Proceedings and arXiv:

37. C. Wang, F. Grillot, V. I. Kovanis, **J. D. Bodyfelt**, J. Even, “Rate Equation Analysis of Frequency Chirp in Optically Injection-Locked Quantum Cascade Lasers”, ed: B. Witzigmann, M. Osinski, F. Henneberger, Y. Arakawa, *Proc. SPIE 8980, Physics and Simulation of Optoelectronic Devices XXII*, 898014 (2014).
38. A. Yafyasov, V. Bogevolnov, A. Tomilov, **B. Pavlov**, G. Fursey, “Modeling of the electron field emission effect on low-dimensional carbon structures”, *Proceedings held in Emission Electronics (ICEE)*, ISBN 9781479956081. Publ. by IEEE, Curran Associate, October 2014, 6 pages.
39. **P. Schwerdtfeger**, O. Ori, **L. Wirz**, J. Avery, “Playing with Hexagons and Pentagons: Topological and Graph Theoretical Aspects of Fullerenes”, *Proceedings of the 14th International Conference on Computational and Mathematical Methods in Science and Engineering*, 2014, 3 pages. DOI: 10.13140/2.1.2307.9042.

### Chapters in Books:

40. **P. Schwerdtfeger**, “Relativity and Chemical Bonding”, in *The Chemical Bond: Fundamental Aspects of Chemical Bonding* (eds. G. Frenking and S. Shaik, Wiley-VCH, Weinheim, 2014); pgs.383-404. ISBN 978-3-527-33314-1.

## 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>



## 2. Conference and Workshop Presentations

### Lectures at Conferences / Meetings:

- J.R. Allison was an invited speaker at the Clusterfest Complex systems meeting, Great Barrier Island, NZ; BIC Biomolecular Computation Symposium, Christchurch, NZ; INMS Postgraduate Conference, Massey University Albany, NZ (keynote); Crystal29, Gold Coast, Australia.
- J.D. Bodyfelt attended the annual March meeting of the American Physical Society in Denver. He gave both an oral presentation and a poster on his flat-band collaborations with S. Flach.
- J. Brand gave a keynote lecture *What can be learned about quantum gases from observing solitary wave dynamics* at the Australasian Workshop for Emergent Quantum Matter, North Stradbroke Island, Australia (December 2014) and gave an invited talk on *Complex solitary waves in constricted superfluids* at Laser Physics Workshop in Sofia, Bulgaria (July 2014).
- Oleksandr Fialko attended the *International Workshop on Laser Physics* in Sofia, Bulgaria (14/07-18/07) and gave an invited talk on *Fate of the false vacuum: towards realization with ultra-cold atoms*.
- S. Flach gave seven lectures/talks at meetings: a keynote lecture at the symposium Nonlinear Wave Phenomena, Technion Haifa, Israel Jan 13; an invited talk at the workshop Weak Chaos and Weak Turbulence, MPIPKS Dresden 03-07 Feb; an invited talk at the conference Disordered Quantum Systems, 19-21 May Paris; an invited lecture at the conference *Let's face chaos through nonlinear dynamics*, Maribor Slovenia June 28 – July 6; an invited lecture at the symposium *Quantum and classical chaos: what comes next?* Ljubljana Slovenia Oct 9-11; a plenary lecture and an invited talk at the 3d *Dynamics Days South America*, Vina del Mar, Chile, Nov 3-7.
- E. Pahl gave invited talks on “*Mercury Melting Simulations: Impact of Relativistic Effects*” at the CMMSE in Cadiz, Spain, on “*Melting of Mercury by parallel tempering Monte Carlo Simulations*” at the International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics in Bratislava, Slovakia and “*Long-Range Correction with MC sampling*” at the Cluster Day on Great Barrier Island, a contributed

talk on “*Influence of Relativistic Effects on the Melting of Mercury*” at the 38<sup>th</sup> Annual Condensed Matter and Materials Meeting on Waiheke Island.

- B. Pavlov gave an invited talk on *A functional model of alternation of modes...* at the *Kent Spectral meeting*. Participation was supported by the organizing committee. University of Kent, April 14 – 17.
- P. Schwerdtfeger gave invited talks on *Toward the Accurate Description of Rare Gas Phases* at the Wagga Meeting in Waiheke, Auckland (February 5); *The Chemistry and Physics of Superheavy Elements* at the American Chemical Society Meeting in Dallas, USA (March 16); a plenary lecture on *The Topology of Fullerenes* at the 14th International Conference Computational and Mathematical Methods in Science and Engineering, Cadiz, Spain (July 3); *Why is Mercury a Liquid at Room Temperature* at the International Conference on Chemical Bonding, Kauai, Hawaii (July 24); *Toward the Accurate Description of Rare Gas Phases* at the 50<sup>th</sup> Symposium of Theoretical Chemistry, Vienna (September 14); *The accurate relativistic electronic structure treatment of superheavy elements with nuclear charge  $Z=111-120$  and beyond*, Relativistic Effects in Heavy Element (REHE) Symposium, Bratislava (September 21); *The wonderful mathematical world of fullerenes* at the Humboldt Colloquium Victoria, Melbourne (October 3).
- Xiaoquan Yu gave a contributed talk at the meeting “Weak Chaos and Weak Turbulence” in Max Planck Institute for the Physics of Complex Systems Dresden, Germany (3 - 7 February 2014), an invited talk at the workshop “Collective Dynamics in Information Systems” in Kavli Institute for Theoretical Physics China at the Chinese Academy of Sciences, Beijing, China. (8-30 October 2014).

## Seminars and Talks:

- J.R. Allison gave invited talks at Griffith University, Australia (two); University of Queensland, Brisbane.
- J. Brand presented a Physics Colloquium with the title *Towards quantum simulation of the early universe with ultra-cold atoms* at the University of Auckland (April 2014), and lectured on *Physics of ultracold Bose gases in one dimension and solitons* at the Victorian Summer School for Ultracold Physics in Melbourne (April 2014).
- S. Flach presented eleven talks: an invited seminar talk at the physics department Tel Aviv University, Jan 16; an invited seminar talk at the Weizman Institute Rehovot, Jan 21.1.14; an invited seminar talk at the math department Massey University Palmerston North April 3; an invited seminar talk at the physics department, University of Regensburg, April 27; an invited seminar talk at the physics department University of Magdeburg, June 24.06; an invited seminar talk at the physics department TU Vienna, June 27; an invited seminar talk at the Université Paris Diderot – Sorbonne Paris Cite October 16; an invited colloquium talk at the Centre Atomico Bariloche Argentina October 31; two CTCP seminar talks Sep 3 and Sep 24; a short INMS presentation on November 28.

- E. Pahl gave a workshop on “*Classical Monte Carlo methods for molecules – write your own MC code to simulate a phase transition*” at the inaugural Quantum and Computational Chemistry Student Conference in June in Christchurch.
- P. Schwerdtfeger gave invited seminars on *High Pressure Physics* at the University of Bonn (January 9); *The Topology of Fullerenes* at INMS Albany (June 6); *The Origin of Biomolecular Homochirality* at the University of the Basque Country (June 30); *The Topology of Fullerenes*, Université Paul Sabatier, Toulouse (July 9); *Beyond the Periodic Table – Going for the Superheavy Elements*, ANU Canberra (October 9).

## Poster Presentations:

- J.R. Allison presented a poster at the International Biophysics Congress, Brisbane, Australia.
- J. Brand and S. Shamilov presented a poster on *Quasiparticles with tunable effective mass: The dispersion relation of atomic Josephson vortices* at the Australasian workshop for emergent quantum matter, Australia (December 2014).
- Jayson G. Cosme presented a poster at the *Australasian Workshop on Emergent Quantum Matter* in Queensland, Australia (3 November).
- Oleksandr Fialko attended the *Australian workshop on emergent quantum matter 2014* in Dunwich, North Stradbroke Island, Australia and presented a poster on *Quantum decay of a relativistic scalar field from a false vacuum: Towards realization with ultracold atoms*.
- E. Pahl gave poster presentations in September on “*Melting of Weakly-Bound Systems by Monte Carlo Simulations*” at the ISSPIC in Fukuoka, Japan and on the Symposium for Theoretical Chemistry in Vienna, Austria.
- S. S. Shamilov presented a poster at the *Australasian Workshop on Emergent Quantum Matter 2014*, held at North Stradbroke Island, Brisbane, Australia.

## 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  
Flatband Physics  
Force Field Parameterisation  
Frequency shifts in atomic clocks  
Graph theoretical and topological properties of fullerenes  
Heterogeneous and Homogeneous Catalysis  
High-Pressure Physics  
Integrated Nanophotonics  
Macroscopic quantum superpositions  
Multiscale Simulation  
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  
Solitonic Vortices  
Spin-dependent parity violation in diatomic molecules  
Stochastic Resonance  
Strongly-correlated fermionic superfluids  
Superheavy Element Chemistry  
Symmetries and Ratchets  
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

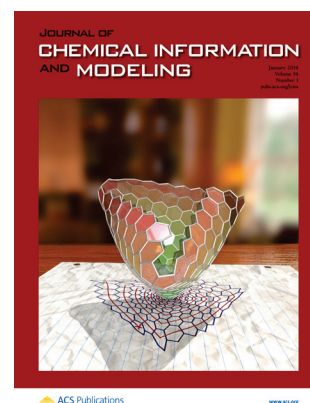
### Honours and Awards:

- J.R. Allison received the *Massey University Early Career Research Medal* and a *Massey University Research Fund Early Career Researcher Award*. She was also the nominated Albany College of Sciences representative at the Royal Society of NZ Early Career Researcher Conference and was accepted for the follow-up RSNZ Early Career Researcher Forum meeting.
- Elke Pahl was promoted to a senior lecturer position.
- P. Schwerdtfeger received the *2014 Rutherford Medal*, the highest award instituted by the Royal Society of New Zealand at the request of the Government to recognise exceptional contributions to the advancement and promotion of public awareness, knowledge and understanding in addition to eminent research or technological practice by a person or group in any field of science, mathematics, social science, or technology. He received the award for his world-leading contributions to fundamental aspects of chemical and physical phenomena in atoms, molecules and condensed matter.
- S. Flach was appointed as director of the Center for Theoretical Physics of Complex Systems, Institute For Basic Science, Daejeon, South Korea.



### Publicity:

- J.R. Allison's Marsden FastStart research was featured on the Royal Society of NZ website (<http://www.royalsociety.org.nz/programmes/funds/marsden/awards/2013-highlights/>) and in the Marsden Fund Update newsletter as a funding highlight. A press release about this was included in NZ Herald article about anniversary of Marsden Fund ([http://www.nzherald.co.nz/nz/news/article.cfm?c\\_id=1&objectid=11204351](http://www.nzherald.co.nz/nz/news/article.cfm?c_id=1&objectid=11204351)). She was also featured in eResearch 2020 discussing long-term ambitions for computational science, in particular data transfer and storage, in New Zealand (<http://ersearch2020.org.nz/opinions/jane-allison-on-hpc-data-options/>)
- S. Flach updated the NZIAS web-site.
- P. Schwerdtfeger and A. Hauser had a title page awarded in the prestigious journal *Angewandte Chemie International Edition* (IF=13.73). Yet another title page was awarded to the fullerene team (Lukas Wirz, James Avery and Peter Schwerdtfeger) by the *ACS Journal of Chemical Information and Modeling* (IF=4.07; see picture to the left). P. Schwerdtfeger had several newspaper articles concerning the Rutherford Medal (New Zealand Herald, Listener, North Sore Times). He also featured on Radio (Saturday Morning National Radio with Kim Hill, and Our Changing World, National Radio). Peter also updated the CTCF website.



## Appendix 4

### POST-GRADUATE SUPERVISION

#### Ongoing PhD Theses:

- Jayson G. Cosme (first year): *Understanding Quantum Thermodynamics in Few-Body Systems*. (Supervisors: J. Brand and O. Fialko)
- Carlo Danieli (second year): *Many-body interactions in quasi-periodic potentials*. (Supervisors: S. Flach, G. Martin, J. Bodyfelt).
- M. Hasanbulli (fourth and last year): *Atoms in Spherical Confinements*. (Supervisors: P. Schwerdtfeger and B. Pavlov). Thesis handed in December 2014.
- A. Punnett (fifth year): *How Hadrons keep their Quarks*. (Supervisor: P. Bowman).
- Sophie Shamailov (first year): *Quantum description of collective nonlinear excitations in bosonic and fermionic cold-atom systems*. (Supervisor: J. Brand)
- Lukas Trombach (first year): *From finite clusters to the solid state: A quantum chemical approach*. (Supervisors: P. Schwerdtfeger and E. Pahl)
- Lukas Wirz (third year): *Computer Modelling of Fullerenes / Biasing molecular modelling with experimental RDCs*. (Supervisors: P. Schwerdtfeger and J.R. Allison)

#### Finished MSc Theses:

none

#### Teaching:

- J. Allison was involved in the papers 246.101, 122.102, 123.172, 246.201 (coordinator), 123.271, 122.231, 122.704 and 162.760.
- J. Bodyfelt lectured on stellar evolution for 124.129 (Astronomy).
- P. Bowman was paper coordinator for 124.226 (Quantum and Statistical Physics), 124.129 (Astronomy) and new paper 124.350 (Computational Physics); taught into 246.102 (Core Skills for Natural Scientists) and 246.302 (Research Themes in Natural Sciences) and delivered special topic 246.301.
- J. Brand is paper coordinator for 124.261 (Nonlinear Physics and Chaos) and taught into 124.102 (Physics 1b), 246.101 (Science and Sustainability).
- S. Flach taught into 124.261 (Nonlinear Physics and Chaos, 18 lectures) and 246.201 (Systems and Models in the Natural Sciences, 9 lectures).
- E. Pahl is paper coordinator of the paper 124.111 – *Physics for Life Sciences* and taught the *Statistical Physics* part of the second year paper 124.226 – *Quantum and Statistical Physics*. (Reduced teaching load due to the MURF woman's award).
- P. Schwerdtfeger gave a lecture course (18 lectures) on *Environmental Chemistry* within the paper *Environmental and Analytical Chemistry* 123.206 (semester 1), and 9 lectures on *Chemical Evolution Theory* for the *Research Themes in Natural Sciences* paper 246.302 (semester 2). He also delivered a summer course (9 lectures) for the Advanced Physical and Computational Chemistry paper 123.331 (semester 3).

## Other activities:

### *Papers refereed:*

- J.R. Allison refereed papers for the journals Nature Scientific Reports, Journal of Molecular Modelling, PLoS One, and Journal of Chemical Theory and Computing. She is also a reviewer for the UK funding bodies EPSRC and BBSRC and A\*STAR (Singapore).
- J. Bodyfelt refereed Europhysics Letters (2 manuscripts) and Physical Review Letters (3 manuscripts). He declined to review three other invitations.
- J. Brand refereed papers for Physical Review Letters, Physical Review A, and New Journal of Physics.
- S. Flach refereed numerous manuscripts for various journals.
- E. Pahl refereed papers for New J. Phys., Chem. Phys. D and Chem. Phys. Lett.
- P. Schwerdtfeger refereed in total 63 papers (rejecting about 2/3 of the invitations) from 21 different international journals including Angewandte Chemie, Nature and Physical Review A.

### *PhD/MSc and other theses refereed:*

- J.R. Allison examined a PhD thesis from the University of Melbourne, and a BSc Hons. thesis from the University of Auckland.
- P. Bowman examined one Honours thesis from the University of Auckland
- J. Brand examined a PhD thesis from the University of Otago.
- Sergej Flach evaluated a master thesis from the University of Auckland, a PhD thesis from Massey University (where he also served as an examiner) and a PhD thesis from the University of Otago.
- P. Schwerdtfeger refereed one PhD thesis from the Indian Institute of Technology, Kharagpur.

### *Conference Organisation:*

- J.R. Allison was part of the organising committee for the Queenstown Molecular Biology meeting, and was nominated to lead the organising committee of a satellite meeting at the 2015 Queenstown Research Week.
- J. Brand, S. Flach and P. Schwerdtfeger organized the NZIAS-MPI tandem workshop on *Nonlinear Physics at the Nanoscale*, Dresden (May 12-16).
- P. Schwerdtfeger was organizer of the symposium on *From Clusters to the Solid State*, 14th International Conference Computational and Mathematical Methods in Science and Engineering, Cadiz, Spain (July 3-7).
- S. Flach and P. Schwerdtfeger organized the 2<sup>nd</sup> NZIAS Xmas Symposium on Complexity in Physics and Chemistry, Albany (December 18).
- S. Flach coordinated a minisymposium at the 3d Dynamics Days South America conference, Vina del Mar (Nov 3-7).

### *Conference Participation:*

- J.R. Allison participated in the Molecular Modelling 2014 and International Biophysics Congress meetings in Australia.
- Jayson G. Cosme attended the Victorian Summer School in Ultracold Physics (VSSUP) in Melbourne, Australia (20-31 January).

### *Chairs at Conferences:*

- J.R. Allison chaired conference sessions at the *Molecular Modelling 2014 and International Biophysics Congress* meetings in Australia.
- J. Brand chaired a session at the Laser Physics workshop in Sofia, Bulgaria (July) and at the NZIAS-MPI tandem workshop on *Nonlinear Physics at the Nanoscale*, Dresden (May 12-16).
- P. Schwerdtfeger chaired sessions at the Wagga Meeting in Waiheke, Auckland (February 4-7), the NZIAS-MPI tandem workshop on *Nonlinear Physics at the Nanoscale*, Dresden (May 12-16), at the *14th International Conference Computational and Mathematical Methods in Science and Engineering*, Cadiz, Spain (July 3), and at the *Relativistic Effects in Heavy Element (REHE) Symposium*, Bratislava (September 24).

### *Boards / Editorial Boards / Professional Societies:*

- J.R. Allison was elected to the committees of the Association of Molecular Modellers of Australasia and the Australian Society for Biophysics.
- P. Schwerdtfeger served on the editorial board *Molecular Physics*, *Journal of Computational Chemistry* and *Computational and Theoretical Chemistry*. He also served on the panel to elect new fellows for the New Zealand Royal Society. He further served on the CoRE selection panel (science, mathematics and engineering). He also served on several MU boards and committees (MU research committee, professorial committee, INMS Exec committee).

### *Community Outreach:*

- J.R. Allison gave seminars at the Biology Olympiad “training camp”, Rotary Science day and Metagenomics high school science event hosted by Massey University, and at Okura High school as part of the Massey University Science Roadshow. She was also invited to contribute to the inaugural Quantum and Computational Chemistry Student Conference (Cass Field Station, NZ).
- P. Bowman gave talks at the Rotary Science day, participated in the Massey Science Research Roadshow at Orewa College, and gave classes as part of Massey@Orewa.
- J. Brand and Physics Staff contributed to a community-engagement session *Kia ora Hauora* for Maori high-school students.
- E. Pahl held physics demonstrations at the Open Day at Massey University, Albany.
- P. Schwerdtfeger gave a public lecture (in German language) on *Das Ende des Periodensystems* at the Max-Planck Institute for Complex Systems, Dresden (May 12).

### *Visits:*

- J.R. Allison visited the research groups of Assist. Prof. Anthony Poole (University of Canterbury), Assist. Prof. Sereina Riniker (ETH Zurich), Prof. Andrew Goodwin (Oxford University), Yaoqi Zhou (Griffith University) and Alan Mark (University of Queensland).
- J. Bodyfelt visited University of Wyoming (his alma mater) and gave a colloquium talk to the physics department.
- S. Flach visited a number of universities in Europe.
- P. Schwerdtfeger visited a number of universities in Europe for potential future research collaborations, including Philipps University Marburg, University of Stuttgart, University of the Basque Country, Université Paul Sabatier in Toulouse, Ottorino Ori’s lab in Parma, and the Australian National University

## 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 2014 (in NZ\$):

### Grants Received/Continuing:

- J. Brand (AI on UoO Marsden grant)	38,000
- Oleksander Fialko (2 <sup>nd</sup> year Marsden FastStart) on “Understanding quantum thermodynamics with the smallest heat engine”.	115,000
- Florian Senn, Swiss Science Foundation	8,250
- E. Pahl (MU Women’s Award)	9,900
- P. Schwerdtfeger (MURF Visitor’s Fund)	1,000
<b>TOTAL</b>	<b>\$ 172,150</b>



## Appendix 5

### Staffing



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

*Joachim Brand, Lukas Trombach, Oleksandr Fialko, Ashar Malik, Jayson G. Cosme, Jane Allison, Lukas Pasteka, Prof. Nikos Lazarides (Visitor), Andrew Punnet, Lukas Wirz, Sophie Shamilov, Xiaoquan Yu, Joshua Bodyfelt, Elisey Kobzev, Ivan Welsh, Elke Pahl, Carlo Danieli, William Irvine, Ali Alavi (Visitor), Boris Pavlov, Gaven Martin (Head of Institute), Patrick Bowman, Sergej Flach, Boris Altschuler (Visitor), Peter Schwerdtfeger.*

*Missing in this picture: Vesna Davidovic-Alexander, Marilou Cadatal-Raduban, Florian Senn, Jonas Wiebke, Mustafa Hasanbulli.*

#### **Personnel:**

Distinguished Prof. Peter Schwerdtfeger (Chemistry, Director of CTCP)

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

Dr. Oleksandr Fialko (Marsden fellow)

Prof. Sergej Flach (Physics)

Prof. Boris Pavlov (Mathematical Physics)

Dr. Jane Allison (Senior Lecturer, Biological Sciences)

Dr. Joshua Bodyfelt (Research Officer)

Dr. Patrick Bowman (Senior Lecturer, Physics)

Dr. Elke Pahl (Senior Lecturer, Physics)

Dr. Marilou Cadatal-Raduban (Senior Tutor, Physics)

#### **Honorary CTCP Members:**

Dr. Anastasia Borschevsky

Dr. Matthias Lein

Dr. Tilo Söhnle

Prof. Uli Zülicke

#### **Secretaries:**

Vesna Davidovic-Alexander (IAS)

Coleen van Es (INMS)

**PhD Students:**

Jayson G. Cosme (Supervisors: J. Brand and O. Fialko)  
Carlo Danieli (Supervisor: S. Flach)  
Mustafa Hasanbulli (Supervisor: P. Schwerdtfeger)  
William Irvine (Supervisor: J. R. Allison)  
Elisey Kobzev (Supervisor: J. R. Allison)  
Ashar Malik (Supervisor: J. R. Allison)  
Andrew Punnett (Supervisor: P. Bowman)  
Sophie Shamilov (Supervisor: J. Brand)  
Lukas Trombach (Supervisors: P. Schwerdtfeger and E. Pahl, started December 2014)  
Ivan Welsh (Supervisor: J. R. Allison)  
Lukas Wirz (Supervisors: P. Schwerdtfeger and J. R. Allison)

**MSc Students:**

none

**Exchange Students:**

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

**Postdoctoral/Research Fellows:**

Dr. Antonio Munoz-Mateo (MU Postdoctoral Fellow)  
Dr. Lukas Pasteka (MU Postdoctoral Fellow)  
Dr. Florian Senn (Swiss Science Foundation, until March 2014)  
Dr. Jonas Wiebke (DAAD fellow and Tutor in Physics, until November 2014)  
Dr. Xiaquan Yu (MU Postdoctoral Fellow)

**Visitors from other institutions:***Long Term:*

Prof. Ali Alavi (MPI Stuttgart and University of Cambridge) visited CTCP in December and delivered two talks on “Quantum Monte-Carlo Theory for Molecules and Solids”.  
Prof. Boris Altshuler (Columbia University) visited CTCP in December to collaborate with S. Flach, and delivered a lecture on “Between localization and ergodicity”.  
Dr. James Avery (Niels Bohr Institute, University of Copenhagen, Denmark), visited CTCP in January to collaborate on the fullerene project.  
Prof. Victor Flambaum and Dr. Julian Berengut (University of New South Wales, Australia) for 1 month in January, both delivered lectures on fundamental problems in physics, and collaborated with P. Schwerdtfeger and A. Borschevsky on nuclear anapole moments and variation of fundamental constants in space-time.

*Short Term for Talks and Collaborations (see CTCP web-site):*

Dr. Nicola Gaston (U Victoria), Prof. Jeff Tallon (U Victoria), Prof. Matt Visscher (U Victoria), Prof. Nikos Lazarides (University of Crete, Heraklion), Prof. John Harvey (U Auckland), Prof. Johannes Richter (Institut für Theoretische Physik, Universität Magdeburg, Germany), Prof. Vladimir Kravtsov (Condensed Matter and Statistical Physics Section, ICTP, Trieste, Italy).