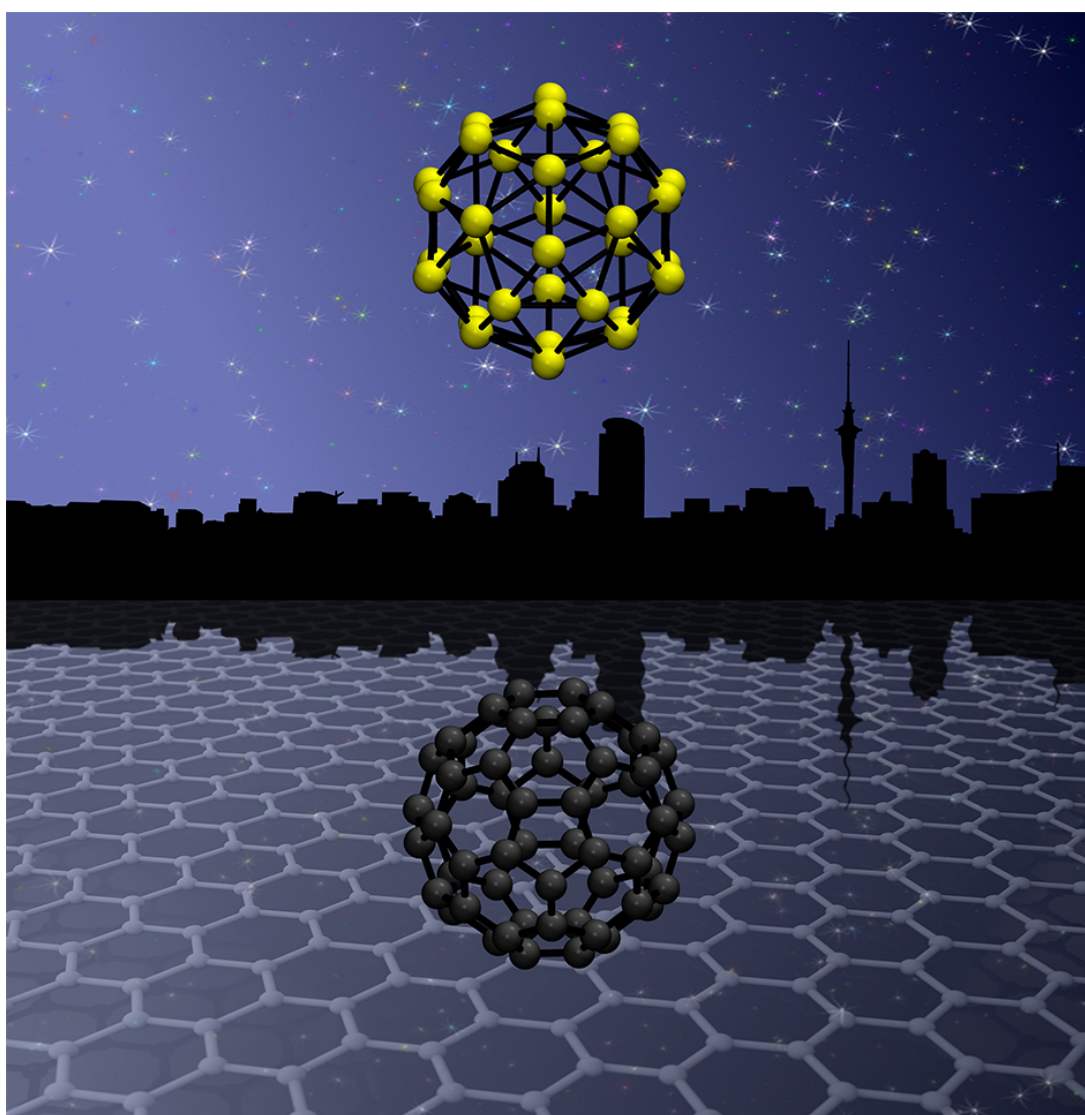


**CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)**  
**NEW ZEALAND INSTITUTE FOR ADVANCED STUDY (NZIAS),**  
**INSTITUTE OF NATURAL AND MATHEMATICAL SCIENCES (INMS)**  
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**2016 MASSEY UNIVERSITY ANNUAL REPORT**  
**CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS**



**Golden Dual Fullerenes** are hollow gold cages that are triangulations of a sphere and topologically isomorph to the well know fullerenes according to Euler's polyhedral formula. This also relates the (111) fcc gold layer to the graphene surface, the gold nanowires to the carbon nanotubes, and the Mackay icosahedra well known in cluster growth simulations to the halma transforms of the fullerene  $C_{20}$ . (L. Trombach, S. Rampino, L.-S. Wang, P. Schwerdtfeger, *Chem. Europ. J.* **22**, 8823 (2016)).

**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 and internationally acclaimed 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 (a new grant was awarded in 2016 to Joachim Brand), four staff are actively involved in the Dodd-Walls CoRE, four others were successful in a funding bid to the Norwegian Centre for Advanced Study (CAS) to perform research in the field of *Chemistry at Extreme Conditions*. Our articles appear regularly in top international journals (this year we had one paper in *Physical Review Letters* and one in *Angewandte Chemie*, both the top journals in their fields). The many high-standing international visitors who joined our research centre in 2016, and the many invitations to international conferences received by our staff, are a clear indication of our success and worldwide recognition.

**Research Output:** This year we published over 30 articles in international journals and books.

**Activities and achievements:** All members of CTCP were actively 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 factors. Sergej Flach continued to run and expand the Centre of Theoretical Physics of Complex Systems as part of the Institute of Basic Science in Daejeon, South Korea. Amongst the outstanding achievements this year were: J.R. Allison received the *Thermofisher Award* for Excellence in Molecular Biology, J. Brand secured a full *Marsden grant* (the only one as PI in the CoS!), and the theoretical chemistry group (E. Pahl, L. Pasteka, P. Schwerdtfeger and K. Steenbergen) is now part of a successful joint collaboration with the Theoretical Chemistry group of T. Helgaker in Oslo, all financed by the Norwegian Centre for Advanced Study. The large number of international eminent visitors we receive each year clearly underlines our international visibility and high level of achievement. In 2016 we had for the first time three postdoctoral fellows financed by the Alexander von Humboldt Foundation, a clear record for New Zealand and only matched by top research institutes in the USA.

**The Future - Opportunities, Risks and Directions:** We are (and continue to be) a top research centre of international high standing. This we achieve despite rather limited financial resources available. The risks are very clear: Other universities overseas are far better resourced, and the loss of excellent staff is inevitable. For example, Prof. Sergej Flach moved to Korea in December 2016. Beside some bureaucratic obstacles typical for a New Zealand University, we are very grateful to MU for the continuous moral and financial support. 2016 was a rather good year for us: our research center is now reasonably well equipped in terms of computational and human resources, and the system management of our CTCP compute cluster improved considerably since Mike Yap took over that difficult task.

**Work in progress:** See attachment for more details.

**Staffing:** Dr. Thomas Engl (Supervisor: S. Flach) and Jan Mewes (Supervisor: P. Schwerdtfeger) joined as Feodor-Lynen Fellows of the Alexander von Humboldt Foundation. Prof. Sergej Flach sadly left us to become director of the Centre of Theoretical Physics of Complex Systems as part of the Institute of Basic Science in Daejeon, Korea. This constitutes a huge loss for our research centre (and the NZIAS), and a new appointment in the area of theoretical sciences is therefore highly desirable.

**Financial:** See Appendix 4.

**Acknowledgment:** The Director is grateful to all CTCP members for their (again) outstanding performance and very hard work in 2016, and wishes everybody an even more successful and productive year 2017. 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 (sometimes demanding) overseas visitors, and organizing us as well (to some success). We acknowledge ongoing support by the Pro-VC Prof. Ray Geor, the HoI INMS Dianne Brunton (for sharing facilities), Dist. Prof. Gaven Martin (for constant advise) and Allan McBride (for financial advise).

A handwritten signature in black ink, appearing to read 'Peter Schwerdtfeger', with a long horizontal stroke extending to the right.

Distinguished Prof. Peter Schwerdtfeger  
Director of CTCP, DHOI NZIAS

**Date:** Tuesday, 20 January 2017

Cc: Prof. Giselle Byrnes (Assistant VC Research, Academic and Enterprise), Prof. Raymond Geor (Pro-VC Science).

## Appendix 1

### Research and Teaching Objectives for 2017

- J. R. Allison will continue the work 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. Elisey will also work on modelling the interaction of anti-microbial peptides with realistic models of the cell membrane, in collaboration with Dr Viji Sarojini (University of Auckland). Ivan will additionally continue his work on improved amino acid-specific dihedral parameters for protein simulations and automated construction of atomic-level force field parameters in collaboration with the group of Prof. Alan Mark at the University of Queensland, which comprise part of the research programme funded by Jane's Rutherford Discovery Fellowship. A third PhD student, Ashar Malik, will continue his work on structural phylogenetics to characterise deep evolutionary relationships, work that is in collaboration with Assoc. Prof. Anthony Poole (University of Canterbury) and also comes under the RDF. William Irvine will continue his PhD work with Jack Flanagan at the Auckland Cancer Research Institute and with Assist. Prof. Joel Tyndall (Otago University) looking at the interactions of proteins with the cell membrane. All four of these students are due to complete in the first half of 2017. Shamim Shadfar, a PhD student funded by the RDF, will work on computational prediction of the selection of bullvalene conformers by cyclodextrins in collaboration with Dr Thomas Fallon (MU). Tom Collier, a postdoctoral research fellow in the Allison group, is also working on the coarse-grained lipid models, as well as modelling the effect of mutations and post-translational modifications on the efficacy of anti-microbial peptides in collaboration with Assoc. Prof. Gill Norris (MU) and Dist. Prof. Margaret Brimble (University of Auckland). Jane will look to continue publishing recent work, and will be hiring a further PhD student to enhance the research capabilities of her group, as well as the capacity to develop new and existing collaborative projects. She will continue her work on designing inhibitors of protein-protein interactions implicated in cancer with INMS staff member Assoc. Prof. Evelyn Sattler, potentially game changing research into the true reason for the temperature-dependence of enzyme activity with Prof. Vic Arcus (Waikato University), and the evaluation of the use of different types of NMR data in concert with molecular dynamics simulations to characterise protein structural ensembles (with Assoc. Prof. Lorna Smith, University of Oxford, and Emiritus Prof. Wilfred van Gunsteren, ETH Zurich).
- P. Bowman is working on the Dirac equation in confining potentials. As well as practical applications to problems in atomic and molecular physics at high pressure there are also interesting mathematical implications in the Dirac equation's (unphysical) tendency to take a continuous spectrum in generic potentials. A new PhD student -- jointly supervised with Dist. Prof. Schwerdtfeger -- will start early in 2017. He has also restarted a project on quark confinement with student Andrew Punnett, which seeks to isolate gauge configurations responsible for quark confinement and dynamical mass generation. Are the same configurations responsible for both properties? That project will be completed early in the year.
- J. Brand will start to work on his Marsden project "Playing dice with Fermi: Full configuration interaction quantum Monte Carlo for fermionic superfluids" with AIs Ali Alavi (Cambridge) and M. Zwierlein (MIT). Another Marsden project and theory-experiment collaboration with the single-atom trapping group of Mikkel Anderson at the University of Otago is finishing this year. The theoretical work on few atom dynamics in an asymmetric double well potential (with Massey graduate student Jayson Cosme) is all

done and the experiment is expected to be completed during 2017. J. Brand will continue his work as Theme Leader for the “Quantum fluids and gases” theme and member of the Executive of the Dodd-Walls Centre for Photonics and Quantum Technologies (a CoRE), where a mid-term review will be completed in 2017. J. Brand is also leading a funded research project on “Quantum emulation and simulation”, which will continue its operations throughout the year. He is currently main supervisor of PhD students Sophie Shamailov, Jayson Cosme, and Peter Jeszinski, with another one expected to start in 2017 and postdoctoral fellows Lauri Toikka, and Antonio Mateo Munoz (starting January 2017). A further postdoctoral fellow will be hired for the Marsden project in the first half of 2017).

- E. Pahl continues to work on the current Marsden project on high-pressure physics/chemistry in collaboration with co-PI Peter Schwerdtfeger. PhD student Odile Smits (Marsden PhD) is now one year into her PhD, working on the melting of heavy rare gas nanoclusters and solids. The necessary ingredients - highly accurate two- and three body potential data are currently computed with high-level quantum-chemical methods and fitted in collaboration with Alexander-von Humboldt postdoctoral fellow Dr Paul Jerabek. First very promising results on ambient-pressure melting of Krypton to super-heavy Oganesson will be published and the studies extended to high pressure. The Marsden postdoctoral fellow Dr Krista Steenbergen works on phase transitions of mercury as well as on the computation of the cohesive energy of super-heavy element Copernicium. Another main project (in collaboration with Peter Schwerdtfeger) lies in the calculation of the so-called Lennard-Jones Ingham coefficients, which will allow an easy computation of cohesive energies, bulk moduli, zero-point energies and other solid-state properties. These computations involve very slowly converging lattice sums, requiring number-theoretical methods – ideas to speed up convergence are mostly developed by now and a manuscript is about to be submitted. Antony Burrows just completed his Honours thesis on this subject and will continue as a PhD student to work on this promising field. A further PhD student Edison Florez will join the high-pressure projects and start early this year. For the second half of the year a sabbatical is planned including an invited two months stay at the Centre for Advance Studies in Oslo, Norway (in the framework of a Norwegian grant) and a stay at the Max-Planck Institute in Stuttgart as a visiting researcher with Prof. Ali Alavi.
- P. Schwerdtfeger will continue work on the 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 with several research groups overseas, namely with Victor V. Flambaum (Sydney) and Anastasia Borschevsky (Groningen) on the variation of fundamental constants in space-time, with Phil Bunker (Ottawa) and Per Jensen (Wuppertal) on Renner-Teller effects in triatomic molecules, and with Richard Mawhorter (Claremont) on electric field gradients in diatomic molecules. Research will also 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. A new Marsden grant will be prepared together with E. Pahl and Witek Nazarewics from Michigan University. Further, there is a commitment to visit Oslo in 2017/2018 as our research center is part of a Norwegian CAS grant on “Molecules in Extreme Environments (MXE)”. For 2017, he is also an invited/plenary speaker at a number of international conferences and meetings overseas, and organizer of a conference on the “Mathematics meets Chemistry – Theoretical Models at the Nanoscale” in Rota, Spain. Two new PhD students will arrive working on several new topics from quantum field theory to cluster modelling. He will also contribute to teaching for the chemistry major in 2016 (environmental chemistry, geochemistry, chemical evolution theory, and introduction to quantum theory for chemists).

## Appendix 2

### 1. Research Output, Publications and Reports

Articles published in 2016 refereed journals (current members of CTCP are in bold letters):

1. **J. R. Allison**, “Let the Powers Combine.” *Structure* **24**, 5-6 (2016).
2. **J. R. Allison**, M. Lechner, M. P. Hoeppe, A. M. Poole, “Positive selection or free to vary? Assessing the functional significance of sequence change using molecular dynamics.” *PLoS One* **11**, e0147619 (2016).
3. **J. G. Cosme**, C. Weiss, **J. Brand**, “Center-of-mass motion as a sensitive convergence test for variational multi-mode quantum dynamics”, *Phys. Rev. A* **94**, 043603 (2016).
4. G. Gligoric, A. Maluckov, Lj. Hadzievski, **S. Flach**, B. Malomed, “Nonlinear localized flatband modes with spin-orbit coupling”, *Phys. Rev. B* **94**, 144302 (2016).
5. D. A. Götz, R. L. Johnston, **P. Schwerdtfeger**, R. Schäfer, “Structural evolution and metallicity of lead clusters”, *Nanoscale* **8**, 11153-11160 (2016).
6. H. Hatami, **C. Danieli**, **J. D. Bodyfelt**, **S. Flach**, “Quasiperiodic driving of Anderson localized waves in one dimension”, *Phys. Rev. E* **93**, 062205 (2016).
7. J. A Harrison, M. A. Sajjad, **P. Schwerdtfeger**, A. J. Nielson, “Multiple Weak C-H Intramolecular Hydrogen Bonding as an Aid to Minimizing Bond Rotation Flexibility”, *Crystal Growth Design* **16**, 4934-4942 (2016).
8. J. A Harrison, A. J. Nielson, M. A. Sajjad, G. C. Saunders, **P. Schwerdtfeger**, “Steric and Electronic Manipulation of the Anagostic Interaction in 1-Tetralone Oxime and Imine Complexes of Rhodium(I)”, *Europ. J. Inorg. Chem.* 64-77 (2016).
9. R. Khomeriki, **S. Flach**, “Landau-Zener Bloch oscillations with perturbed flat bands”, *Phys. Rev. Lett.* **116**, 245301 (2016).
10. Y. Kominis, T. Bountis, **S. Flach**, “The Asymmetric Active Coupler: Stable Nonlinear Supermodes and Directed Transport”, *Scientific Reports* **6**, 33699 (2016).
11. J. Lee, N. Joshi, R. Pasini, R. C. J. Dobson, **J. R. Allison**, T. Leustek, “Inhibition of Arabidopsis growth by the allelopathic compound azetidine 2-carboxylate is due to the low amino acid specificity of cytosolic prolyl-tRNA synthetase.” *Plant J.* **88**, 236-246 (2016).
12. R. Liao, **O. Fialko**, **J. Brand**, U. Zülicke, “Noncollinear drag force in Bose-Einstein condensates with Weyl spin-orbit coupling”, *Phys. Rev. A* **93**, 023625 (2016).
13. Y. Minami, R. Arita, **M. Cadatal-Raduban**, M. H. Pham, M. J. F. Empizo, M. V. Luong, T. Hori, M. Takabatake, K. Fukuda, K. Mori, K. Yamanoi, T. Shimizu, N. Sarukura, K. Fukuda, N. Kawaguchi, Y. Yokota, A. Yoshikawa, “Temperature-dependent evaluation of Nd:LiCAF optical properties as potential vacuum ultraviolet laser material”, *Opt. Mat.* **58**, 5-8 (2016).
14. B. Ostojić, **P. Schwerdtfeger**, P. Jensen, P. R. Bunker, “An ab initio study of SbH<sub>2</sub> and BiH<sub>2</sub>: The Renner Effect, Spin-Orbit Coupling, Local Mode Vibrations and Rovibronic Energy Level Clustering”, *J. Mol. Spectr.* **330**, 130-141 (2016). (dedicated to Robert Le Roy).
15. **L. F. Pašteka**, R. J. Mawhorter, **P. Schwerdtfeger**, “Relativistic Coupled-Cluster Calculations of the <sup>173</sup>Yb Nuclear Quadrupole Coupling Constant for the YbF Molecule”, *Mol. Phys.* **114**, 1110-1117 (2016).

16. T. Pichugina, T. Sugawara, A. Kaykov, W. Schierding, K. Masuda, J. Uewaki, R. S. Grand, J. R. **Allison**, **R. A.** Martienssen, P. Nurse, M. Ueno, J. M. O'Sullivan, "A diffusion model for the coordination of DNA replication in *Schizosaccharomyces pombe*." *Nat. Sci. Rep.* **6**, 18757 (2016).
17. **P. Schwerdtfeger**, R. Tonner, G. A. Moyano, **E. Pahl**, "Towards J/mol Accuracy for the Cohesive Energy of Solid Argon", *Angew. Chem. Int. Ed.* **55**, 12200-12205 (2016); *Angew. Chem.* **128**, 12387-12392 (2016).
18. **S. S. Shamailov**, **J. Brand**, "Dark-soliton-like excitations in the Yang–Gaudin gas of attractively interacting fermions", *New J. Phys.* **18**, 075004 (2016).
19. **K.G. Steenbergen**, N. Gaston. "A 2D liquid structure explains the elevated melting temperatures of gallium nanoclusters", *Nano Lett.* **16**, 21-26 (2016).
20. **K.G. Steenbergen**, J.L. Kern, Z. Wang, W.H. Thompson, B.B. Laird. "Tunability of Gas-Expanded Liquids Under Confinement: Phase Equilibrium and Transport Properties of Ethylene-Expanded Methanol in Mesoporous Silica", *J. Phys. Chem. C* **120**, 5010–5019 (2016).
21. **L. Trombach**, S. Rampino, L.-S. Wang, **P. Schwerdtfeger**, "Hollow Gold Cages and their Topological Relationship to Dual Fullerenes", *Chem. Europ. J.* **22**, 8823-8834 (2016). (selected as hot paper with cover page; dedicated to Prof. G. Frenking's 70<sup>th</sup> birthday).
22. L. Wirz, R. Sure, R. Tonner, A. Hermann, **P. Schwerdtfeger**, "A Harmonic Force-Field Method for Fullerenes and a Comparison to Density Functional Calculations for Goldberg-Coxeter Fullerenes up to C<sub>980</sub>", *J. Comput. Chem.* **37**, 10-17 (2016).
23. Zare, D., **Allison**, **J.R.**, McGrath, K.M. "Molecular dynamics simulation of  $\beta$ -lactoglobulin at different oil/water interfaces." *Biomacromol.* **17**, 1572-1582 (2016).
24. P. Zou, **J. Brand**, X.-J. Liu, H. Hu, "Traveling Majorana Solitons in a Low-Dimensional Spin-Orbit-Coupled Fermi Superfluid", *Phys. Rev. Lett.* **117**, 225302 (2016).

## Refereed Conference Proceedings and arXiv:

25. P. D. Drummond, **J. Brand**, "Comment on: 'Single-shot simulations of dynamic quantum many-body systems'", arXiv:1610.07633 (2016).
26. **O. Fialko**, B. Opanchuk, A. I. Sidorov, P. D. Drummond, **J. Brand**, "The universe on a table top: engineering quantum decay of a relativistic scalar field from a metastable vacuum", arXiv:1607.01460 (Journal of Physics B, in print).
27. **S. Flach**, R.Khomeriki, "Fractional lattice charge transport ", arXiv:1606.03703. (Scientific Reports, in print).
28. D. Leykam, **J. D. Bodyfelt**, A. S. Desyatnikov, **S. Flach**, "Localization of weakly disordered flat band states", arXiv:1601.03784. (European Physical Journal B, in print).
29. **P. Schwerdtfeger**, "Toward an accurate description of solid-state properties of superheavy elements. A case study for the element Og (Z=118)", *EPJ Web Conf.* **131**, 07004-1-6 (2016) (invited paper).
30. **L. A. Toikka**, **J. Brand**, Exactly solvable model for a solitonic vortex in a compressible superfluid, (2016). arXiv: 1608.08701
31. S.-W. Su, I.-K. Liu, S.-C. Gou, R. Liao, **O. Fialko**, **J. Brand**, "Hidden long-range order in a two-dimensional spin-orbit coupled Bose gas", arXiv:1609.05464 (2016).



## Chapters in Books:

32. A. W. Hauser, **P. Schwerdtfeger**, "Nanoporous graphene sheets for gas separation", *Graphene Science Handbook* (M. Aliofkhazraei, N. Ali, W. I. Milne, C. S. Ozkan, S. Mitura, J. L. Gervasoni (Eds.), CRC Press, Taylor & Francis, 2016); chapter 25, pgs. 473-486.
33. **S. Flach**, "Spreading, Nonergodicity, and Selftrapping: A Puzzle of Interacting Disordered Lattice Waves", Springer International Publishing Switzerland 2016 1 M. Tlidi and M. G. Clerc (eds.), *Nonlinear Dynamics: Materials, Theory and Experiment, Springer Proceedings in Physics*, 173, DOI 10.1007/978-3-319-24871-4\_3.

## Software developments:

- P. Schwerdtfeger**, L. Wirz and J. Avery: Software package *Fullerene Version 4.5*, released November 2015, available under open source and can be found online at CTCP, Massey University, Albany. Web-site at <http://ctcp.massey.ac.nz/index.php?group=&page=fullerenes&menu=fullerenes>
- P. Schwerdtfeger**, Program LatticeSum: A Fortran program to calculate lattice sums for cubic and hexagonal closed packed lattices.



## 2. Conference and Workshop Presentations

### Lectures at Conferences / Meetings:

- J.R. Allison gave a keynote lecture at the RACI Physical Chemistry Meeting, Christchurch, New Zealand; contributed talks at the Lorne Proteins meeting, Australia and at the Crystal30 meeting, Hobart, Australia; an invited talk at the NZ Institute of Chemistry meeting, Queenstown, New Zealand; the Excellence in Molecular Biology Research Award talk at the Queenstown Molecular Biology meeting, Nelson, New Zealand; and was an invited panel member for a discussion on the Future of Science in New Zealand at the NZ Association of Scientists meeting, Wellington, New Zealand. She was also invited to speak at Multicore World, Wellington, NZ, and at the Biophysical Society meeting, Berlin, Germany, but declined due to prior commitments.
- J. Brand gave invited talks at the workshop "Topological Effects in Ultra-Cold Atoms" in Natal, Brazil (Nov 2016), at the workshop "Control of light and matter wave propagation and localization in photonic lattices" in Santiago de Chile (Nov 2016), the Matariki workshop on Quantum Science in Dunedin (March 2016), and at the 2016 Xmas Theoretical Physics Symposium in Wellington.
- O. Fialko gave an invited talk on "Fate of the false vacuum: towards realization with ultra-cold atoms" at the NZIAS-MPIPES Return Tandem Workshop on Nonlinear Physics at the Nanoscale, Rotorua, New Zealand (Feb 2015); contributed talk on "Towards an isolated quantum heat engine" at the NZIP Conference celebrating "The International Year of Light", Hamilton, New Zealand (Jul 2015); Contributed talk on "Engineering Quantum Decay of a Relativistic Scalar Field From a False Vacuum via Periodically Driving Coupled Condensates" at the International Workshop on Laser Physics, Shanghai,



China (Aug 2015).

- S. Flach gave twelve (12) invited lectures/talks at meetings: APS March Meeting 2016, March 14-18 2016, Baltimore USA; Recent progress and perspectives in topological insulators: quantum Hall effects, ballistic vs. diffusive regimes and Anderson transitions KITPC Beijing China, April 11-29 2016; The Dynamics of Complex Systems: A meeting in honour of the 60th birthday of Robert MacKay FRS, Wawrick UK, 18-20 May 2016; 617. WE-Heraeus-Seminar: Quantifying Complex Transport with Levy Walks: From Cold Atoms to Humans and Robots Physikzentrum Bad Honnef, Germany, May 23 - 27 2016; NetSci, Seoul, South Korea, May 30 - June 3 2016; 10th International Workshop on Disordered Systems, Brescia Italy, June 27 - July 1 2016; Disorder, Interactions and Coherence: Warps and Delights International focus workshop. MPIPKS Dresden Germany, 13 - 15 July 2016; Workshop on Analysis and Applications of Localized Structures in Nonlinear Media, Lorentz Center Leiden The Netherlands, Aug 29 - Sep 2 2016; 3rd Dynamics Days Central Asia, Astana Kazakhstan, Sep 2-5 2016; Dynamics Days Latin America and the Caribbean, Puebla, Mexico, October 24 - November 01, 2016; and DDAP9: 9th Dynamics Days Asia-Pacific, Hong Kong, Dec. 14-17, 2016.
- P. Jerabek gave an invited talk on "Insights into the Bonding Situation of Interstitially Stabilized Gold Clusters" at the [CMMSE'16](#), Rota, Spain (Jul 2016); contributed talk on "The Nitrate-Peroxonitrite Isomerization Reaction Mechanism" at the NZIC-2016, Queenstown, New Zealand (Aug 2016); keynote on "Obtaining Highly Accurate Many Body Potentials for Heavy and Superheavy Rare Gas Clusters" at Cluster Symposium 2016, Christchurch, New Zealand (Dec 2016).
- A. Malik gave talks titled "The truth is out there ..." at the First NZ Astrobiology conference, Kaikoura, New Zealand (January 2016); "Exploring Deep Phylogenies using Protein Structure" at The 20th Annual New Zealand Phylogenomics Meeting, Mount Ruapehu, North Island, New Zealand (February 2016); "Exploring Deep Phylogenies using Protein Structure" at QUACCS2.0, Cass field station, University of Canterbury, New Zealand (June 2016).
- E. Pahl gave a talk on "Au/Pd nanocluster as catalysts" at AMN-7, Nelson, New Zealand (February 2016), an invited talk titled "Argon Melting under High Pressure" at the 16th International Conference on "Computational and Mathematical Methods in Science and Engineering" in Cadiz, Spain (July 2016) and a talk on "Phase Transitions of Argon under High Pressure" at the NZIC in Queenstown in August 2016 and gave a keynote presentation on "Rare Gas Problems" at the Cluster symposium in Christchurch in November. In June, Elke participated in the second QUACCS winter school, delivering workshops on "Introduction into Monte Carlo Methods".
- L. F. Pašteka gave a talk titled "Search for variation of fundamental constants" at the 2016 New Zealand Institute of Chemistry Conference (Queenstown).
- P. Schwerdtfeger gave a keynote lecture on *From Graphene to Graphyne, Fullerenes, Fulleroids, Gaudienes and their Golden Duals* within the carbon materials section at the 7th Asia Pacific Conference of Theoretical and Computational Chemistry (APCTCC7), Kaohsiung, Taiwan, January 25-28, 2016; a plenary lecture on *From Graphene to Graphyne, Fullerenes, Fulleroids, Gaudienes and their Golden Duals* at the RACI Physical Chemistry Meeting 2016, Christchurch, February 2 – 5, 2016; a keynote lecture on *Toward an Accurate Description of Chemical and Physical Properties of the Superheavy Elements*, Nobel Foundation Symposium on Superheavy Elements at the Bäckaskog Castle, Sweden, May 29 – June 2; a plenary lecture on *From graphene to graphyne, fullerenes, fulleroides, gaudienes and their golden duals* at the International Conference on Modern Aspects of Structural Chemistry, June 5-7, Ulm, Germany; an invited lecture on *The Lennard-Jones Potential Revisited: Analytical Solutions for the Solid State from Lattice Sums and Epstein Zeta Functions* at the CMMSE2016, 15th International Conference on "Computational and Mathematical Methods in Science and

Engineering”, Cadiz (Spain), July 4-8, 2016; invited talk on *Semi-Local All-Electron Effective Potentials for Quantum Electrodynamical Effects in 4- and 2-Component Relativistic Theories* at the Congress Of The International Society Of Theoretical Chemical Physics 2016, Grand Forks, North Dakota, USA, July 17-22, 2016; a plenary lecture on *Left or Right in Nature – The Search for Breakdown of Chiral Symmetry in Molecules* at the NZIC Chemistry Conference in Queenstown, August 21-24, 2016; a keynote lecture on *The Lennard-Jones Potential Revisited: Analytical Solutions for the Solid State from Lattice Sums and Epstein Zeta Functions* at the Computational Chemistry Meeting, Perth, December 1-2, 2016.

- K. G. Steenbergen gave talks at (i) the 2016 *Royal Australian Chemical Institute Physical Chemistry Meeting* (Christchurch), (ii) the 16<sup>th</sup> *International Conference Computational and Mathematical Methods in Science and Engineering* (Rota, Spain), (iii) the 2016 *New Zealand Institute of Chemistry Conference* (Queenstown), (iv) an invited talk at the 2016 *MacDiarmid Theory Meeting* (Leigh), and (v) the *Cluster Symposium 2016* (Christchurch).
- Lauri A. Toikka gave a talk at the DWC Symposium in Queenstown on the newly developed asymptotically solvable hydrodynamical model for tightly-confined vortices.
- L. Trombach gave talks on the relationship between hollow gold clusters and fullerenes at the 16<sup>th</sup> *international conference CMMSE* (Rota, Spain) and the *NZIC conference* (Queenstown, New Zealand). He also gave an invited talk titled “From Kissing Spheres to Lennard-Jones Clusters” at the 14<sup>th</sup> *Annual Clusters and Nanoparticles meeting* (Christchurch, New Zealand).
- I. Welsh gave a talk titled “Automated parameterisation of the world” at the INMS postgraduate conference (October 2016).

## Seminars and Talks:

- J.R. Allison gave talks at the University of Queensland, Brisbane, Australia; Massey University, Palmerston North, New Zealand; University of Canterbury, New Zealand.
- P. Bowman gave a talk on properties of the Dirac equation at the INMS weekly seminar.
- J. Brand gave a talk titled “Towards quantum Monte Carlo for ultracold atoms or: how to solve a computational problem that is way too big” at Massey University (Sept 2016).
- T. Engl gave a talk on "Universal Many-Body Interference beyond Mean-Field Theory in Fock Space" (June 13 - 24, Daejeon, South Korea).
- S. Flach presented four talks: one at Boston University, one at Massey University, two at IBS Daejeon.
- P. Jerabek gave a seminar on "Exploring Potential Energy Surfaces and Excited States" at Chemistry Department of University of North Texas, Denton, USA (Jul 2016); a hands-on workshop on "Investigating Chemical Bonding with ADF" (5 hours, 25 participants) at Chemistry Department of University of North Texas, Denton, USA (Jul 2016); seminar on "The Nitrate-Peroxonitrite Isomerization Reaction Mechanism" at INMS seminar (Nov 2016).
- E. Kobzev gave talks titled “Coarse-grain lipids” at ETH Zürich, Switzerland and the University of Southampton, UK (May 2016)
- E. Pahl held a seminar talk on “Melting of Nanoclusters and Extended Systems” at the University of Heidelberg, Germany and an NZIAS/INMS seminar talk on “Rare Gas Problems” in August.
- L. F. Pašteka gave a talk on *Variation of fundamental constants in space-time* at Malmö University, Sweden and at Massey University within the NZIAS/INMS Friday seminar series.
- P. Schwerdtfeger gave four talks at Wayne State University (Detroit) in 2016: The

Frontiers in Chemistry talk on *Left or Right in Nature - Biomolecular Homochirality and Chemical Evolution*, April 4, on *The Topology of Fullerenes*, Department of Mathematics, April 5, on *Space-Time Variation of Fundamental Constants*, Department of Physics, April 5, *High Pressure Simulations of Atoms and Molecules*, Department of Chemistry, April 6. Additional seminars delivered: *The Variation of Fundamental Constants in Space-Time*, Physics Department, Johannes Gutenberg University of Mainz, Mainz, April 21; *Playing with Pentagons and Hexagons – The Wonderful World of Fullerenes*, LMU Munich, April 27; *The Topology of Fullerenes*, Max-Planck Institute of Solid-State Physics, Stuttgart, May 4; *Relativistic Effects in the Chemistry and Physics of Gold*, Department of Materials Science, University of Milano-Bicocca, Milano, Italy, June 29; short talk on *There is a Hole in my Membrane* at the INMS weekly seminar, Albany, September 16; *Playing with Pentagons and Hexagons – The Wonderful World of Fullerenes* at the AUT, Auckland, October 6; seminar on *The Theory of Pseudopotentials*, Massey University Albany, October 21;

- K.G. Steenbergen gave a talk at Massey University (INMS seminar).
- O. Smits gave a talk titled “Tell me your secret, Oganesson, are you a liquid or a solid at room temperature?” at the INMS postgraduate conference (October 2016). She was the winner of the Best Speaker Award.
- Lauri A. Toikka gave talks on solitonic vortices at the Institute for Basic Science, KAIST (Daejeon, South Korea), Matariki Workshop on Quantum Science (Dunedin, New Zealand), and Turku Centre for Quantum Physics, University of Turku (Finland).

## Poster Presentations:

- J. Brand presented a poster at the OSA Nonlinear Photonics meeting in Sydney (Sep. 2016) where he also served on the programme committee.
- Jayson G. Cosme presented a poster on “Breakdown of standard test in detecting slow convergence of variational multi-mode quantum dynamics of attractive bosons”, at MQS2016: Matariki Workshop on Quantum Science, Dunedin, New Zealand, March 2016.
- Carlo Danieli presented a poster at DDAP9: 9th Dynamics Days Asia-Pacific, Hong Kong, Dec. 14-17, 2016. Poster: Quasiperiodic driving of Anderson localized waves in one dimension.
- T. Engl presented posters in Brescia, Italy: Poster: "Many-body Spin Echo" (June 25 - July 1) and in Dresden, Germany: Poster "Many-body Spin Echo" (July 13 -15),
- W. Irvine presented a poster titled “Computational Characterisation of Protein-Membrane Interactions” at the Drug Discovery satellite meeting (August 2016) and the Queenstown Molecular Biology meeting (September 2016), where he also gave a lightening talk to promote his poster. He also presented a poster with the same title at the INMS postgraduate conference (October 2016).
- P. Jerabek presented a poster titled "Understanding F 1s NEXAFS Dichroism in Perfluoropentacene" at ISTCP-2016, Grand Forks (ND), USA (Jul 2016)
- E. Kobzev presented a poster titled “Coarse-graining of lipids” at the INMS postgraduate conference (October 2016).
- O. Smits presented a poster titled “ Importance of an accurate potential on the melting temperature of noble gas cluster” at the NZ Institute of Chemistry meeting (June 2016).
- Lauri A. Toikka presented a poster at ICAP (Seoul, South Korea).
- L. Trombach presented a poster at the *RACI Physical Chemistry Meeting* (Christchurch, New Zealand).
- I. Welsh presented a poster titled “Automated parameterisation of the world” at the NZ Institute of Chemistry meeting (June 2016).

## Appendix 3

### 1. RESEARCH

#### **Current Areas of Research Activities:**

Biomolecular Simulations  
Cayley-Dickson Interpretations of Physics  
Celestial Mechanics  
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  
Lattice Sums for extended systems  
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  
Optical properties for VUV lasers  
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 Monte Carlo simulations of fermionic superfluids  
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 has been awarded the Thermofisher Award for Excellence in Molecular Biology.

### Publicity:

- J.R. Allison and collaborators had a cover page awarded for their review article “Deriving structural information from experimentally measured data on biomolecules: a review.” published in the high profile journal *Angewandte Chemie*: van Gunsteren, W.F., Allison, J.R., Daura, X., Dolenc, J., Hansen, N., Mark, A.E., Oostenbrink, C., Rusu, V.H., Smith, L.J. “Deriving structural information from experimentally measured data on biomolecules: a review.” *Angew. Chem.* (in press, DOI: 10.1002/anie.201601828). Her research was featured in a case study on the use of NeSI resources: <https://www.nesi.org.nz/case-studies/new-frontiers-milk-proteins-functional-foods-and-drug-delivery-systems>. She was also featured in the Curious Minds Women in STEM series: <http://www.curiousminds.nz/about/jane-allison/>
- P. Schwerdtfeger and L. Trombach had a title page awarded for Chemistry – A European Journal. The paper was also selected as a hot paper by the journal. Peter was interviewed by North Shore Times on *Why Is the Universe Left-handed? But Humans Don't Tend to Be*, September 22 (appeared also in New Zealand Herald). Peter also appeared on Radio NZ with Jesse Mulligan discussing the topic *Why the Universe is structured to be left handed*, 2:30 pm on 26 September 2016.

## Appendix 4

### POST-GRADUATE SUPERVISION

#### Ongoing PhD Theses:

- Jayson G. Cosme (second year): *Understanding Quantum Thermodynamics in Few-Body Systems*. (Supervisors: J. Brand and O. Fialko).
- Carlo Danieli (third year): *Advances in classical and quantum wave dynamics on quasiperiodic lattices*. (Supervisors: S. Flach, G. Martin, J. Bodyfelt). Successfully finished.
- William Irvine (third year): *Proteins, membranes and diseases: a computational approach*. (Supervisors: J.R. Allison, J.U. Flanagan (U. Auckland) and P. Schwerdtfeger).
- Péter Jeszenszki (first year). Supervisor: J. Brand.
- Yağmur Kati (first year): *Space-Time Correlations for Nonergodic Disordered Nonlinear Waves*. (Supervisors: S. Flach, P. Schwerdtfeger, J. Bodyfelt).
- Elisey Kobzev (third year): *Development and application of multiscale models for biomolecular simulation*. (Supervisors: J.R. Allison and P. Schwerdtfeger).
- Ashar Malik (third year): *The evolution of phylogenetics: from sequence to structure*. (Supervisors: J.R. Allison, A.M. Poole (U. Canterbury) and P. Schwerdtfeger).
- Andrew Punnett (sixth year): *How Hadrons keep their Quarks*. (Supervisor: P. Bowman).
- Shamim Shadfar (first year): *Molecular dynamics simulation of inter-molecular interactions* (Supervisors: J.R. Allison and T. Fallon)
- Sophie Shamailov (third year): *Quantum description of collective nonlinear excitations in bosonic and fermionic cold-atom systems*. (Supervisor: J. Brand)
- Odile Smits (first year): *The solid-to-liquid phase transitions in heavy rare gas systems*. (Supervisors: P. Schwerdtfeger and E. Pahl)
- Lukas Trombach (second year): *From finite clusters to the solid state: A quantum chemical approach*. (Supervisors: P. Schwerdtfeger and E. Pahl)
- Ivan Welsh (third year): *Automated parameterisation of the world\**. (Supervisors: J.R. Allison and P. Schwerdtfeger)

#### Finished PhD Theses:

- Carlo Danieli: *Advances in classical and quantum wave dynamics on quasiperiodic lattices*. (Supervisors: S. Flach, G. Martin, J. Bodyfelt).

#### Finished Honors Theses:

- Antony Burrows: *On the Calculation of Lennard-Jones-Ingham Coefficients to High Accuracy for Cubic and Hexagonal Lattices*. (Supervisors: E. Pahl, P. Schwerdtfeger).

#### Teaching:

- J.R. Allison was involved in the papers 246.201 (coordinator), 123.271 and 122.704.
- J. Bodyfelt lectured on stellar evolution for 124.129 (Astronomy).
- P. Bowman was paper coordinator for 124.171 and 124.172 (Physical Principles for Engineering and Technology I & II), 124.226 (Quantum and Statistical Physics) and 124.129 (Astronomy); and taught into 246.102 (Core Skills for Natural Scientists).

- J. Brand is paper coordinator for 124.261 (Nonlinear Physics and Chaos) and also taught into 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 first half of this paper. She also taught the Statistical Physics part (6 weeks) of the 124.226 Quantum and Statistical Physics paper.
- P. Schwerdtfeger gave lecture courses (15 lectures) on *Environmental Chemistry* within the paper *Environmental and Analytical Chemistry* 123.206 (semester 1), *Introduction to Quantum Theory* (15 lectures) for the *Advanced Physical and Computational Chemistry paper* 123.331 (semester 1).

## Other activities:

### *Papers refereed:*

- J.R. Allison refereed papers for the journals *Structure*, *Scientific Reports*, *European Biophysics Journal*, *Journal of Chemical Theory and Computation*, *PhysChemChemPhys*, *PLoS One*, *Progress in Biophysics and Molecular Biology*
- J. Brand refereed papers for *Science*, *Scientific Reports*, *Physical Review Letters*, *Physical Review A* and *Journal of Physics B*. In addition he reviewed fellowship proposals for the Research Foundation Flanders (FWO) and the Alexander von Humboldt Foundation.
- P. Jerabek refereed papers for *Journal of Computational Chemistry*
- E. Pahl refereed papers for *JACS* and the *Journal of Physical Chemistry*.
- P. Schwerdtfeger refereed in total 42 papers (rejecting about 2/3 of the invitations) from 25 different international journals including *Angewandte Chemie*, *Nature*, *Physical Review Letters* and *J. Am. Chem. Soc.*
- S. S. Shamailov refereed a paper for the *Journal of Physics B: Atomic, Molecular and Optical Physics*.
- K.G. Steenbergen refereed papers for the journals *Computational Materials Science* and the *Journal of Physical Chemistry*.
- L. A. Toikka refereed in total around 10 papers for *J. Phys. B: At. Mol. Opt. Phys*, *New Journal of Physics*, *Physical Review A*, and *Phys. Lett. A*.

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

- J.R. Allison examined the PhD theses of Amy Xu (School of Chemical Sciences, University of Auckland), Eric Lang (Department of Chemistry, University of Canterbury), Nathaniel Gunby (Department of Chemistry, University of Canterbury), Tamara Betancur (Research School of Chemistry, Australian National University), Toni Daly (IFS, Massey University), Yuriy Pichugin (NZIAS, Massey University); the PhD confirmation of Elena Denisoko (INMS, Massey University); and the BSc Hons thesis of Hugh Glossop (School of Chemical Sciences, University of Auckland).
- P. Bowman examined one PhD thesis from Massey University.
- J. Brand examined the PhD theses of Jan Zill (University of Queensland) and Yin Hsien Fung (University of Otago). He further served as convenor for the confirmation of Yagmur Kati (Massey).



#### *Graduate Summer School Organisation:*

- J.R. Allison contributed to the biennial Quantum Computational Chemistry Student Conference (Quaccs, <https://quaccs.wordpress.com/>), Cass, New Zealand.
- E. Pahl contributed to the biennial Quantum Computational Chemistry Student Conference (Quaccs, <https://quaccs.wordpress.com/>), Cass, New Zealand.
- I. Welsh contributed to the biennial Quantum Computational Chemistry Student Conference (Quaccs, <https://quaccs.wordpress.com/>), Cass, New Zealand.

#### *Conference Organisation:*

- J.R. Allison organised the Queenstown Molecular Biology meeting, Nelson, New Zealand.
- J. Brand organised a retreat for the investigators of the Quantum Fluids and Gases theme of the Dodd-Walls Centre in Wellington 27-28 October 2016.
- P. Schwerdtfeger was part of the organizing committee for the CMMSE2016, 15th International Conference on “Computational and Mathematical Methods in Science and Engineering”, Cadiz (Spain), July 4-8, 2016.

#### *Conference Participation:*

- J.R. Allison attended the KiwiFoo Unconference, New Zealand (invitation only); Society for Molecular Biology and Evolution, Gold Coast, Australia; Drug Discovery, Nelson, New Zealand; NZ Society for Biochemistry and Molecular Biology, Christchurch, New Zealand; Biomolecular Interaction Centre symposium, Christchurch, New Zealand; Maurice Wilkins Centre annual symposium, Auckland New Zealand.
- K. G. Steenbergen attended RACI Physical Chemistry Meeting, CMMSE and NZIC.
- L. Toikka participated in ICAP (Seoul, South Korea), DWC Symposium (Queenstown), and the Matariki Workshop on Quantum Science (Dunedin).
- L. Trombach attended RACI Physical Chemistry Meeting, CMMSE and NZIC.

#### *Chairs at Conferences:*

- J.R. Allison chaired sessions at the Lorne Proteins meeting, Australia; RACI Physical Chemistry meeting, Christchurch, New Zealand; NZ Institute of Chemistry meeting, Queenstown, New Zealand; Queenstown Molecular Biology meeting, Nelson, New Zealand.
- J. Brand chaired sessions at the Dodd-Walls Symposium in Queenstown (June 2016), at the workshop “Topological Effects in Ultra-Cold Atoms” in Natal, Brazil (Nov 2016), at the workshop “Control of light and matter wave propagation and localization in photonic lattices” in Santiago de Chile (Nov 2016), and at the Matariki workshop on Quantum Science in Dunedin (March 2016).
- E. Pahl chaired sessions at the RACI Physical Chemistry meeting, Christchurch, New Zealand and the Cluster Symposium in Christchurch, New Zealand.
- P. Schwerdtfeger chaired sessions at the 7th Asia Pacific Conference of Theoretical and Computational Chemistry (APCTCC7), Kaohsiung, Taiwan, January 25-28; at the RACI Physical Chemistry Meeting 2016, Christchurch, February 2 – 5, 2016; at the CMMSE2016, 15th International Conference on “Computational and Mathematical Methods in Science and Engineering”, Cadiz (Spain), July 4-8, 2016; at the Congress Of The International Society Of Theoretical Chemical Physics 2016, Grand Forks, North Dakota, USA, July 17-22, 2016; at the NZIC Chemistry Conference in Queenstown, August 21-24, 2016.

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

- J.R. Allison is the chair of the Royal Society of New Zealand Early Career Researcher Forum; a member of the RSNZ Gene Editing Expert Advice Panel; the NZ representative on the committees of the Australasian Biophysics Society and the Association of Molecular Modellers of Australasia; the sub-professorial representative on the INMS Executive Committee, the INMS representative on the Massey University College of Sciences Research Committee; an early career representative on the Massey University Research Committee; a member of the Massey University Research Data Management Committee; the Massey University New eScience Infrastructure liaison person. She is an Associate Investigator at the Biomolecular Interaction Centre (University of Canterbury) and the Maurice Wilkins Centre for Molecular Biodiscovery. She is a member of the Royal Society of New Zealand; Society of Crystallographers of Australia and New Zealand; New Zealand Association of Scientists; New Zealand Society for Biochemistry and Molecular Biology.
- J. Brand served as member of the Executive Committee, as member of the Science Team and as Theme Leader for the theme Quantum Fluids and Gases of the Dodd-Walls Centre for Photonic and Quantum Technologies. He was also on the programme committee for the OSA conference Nonlinear Photonics in Sydney (Sept. 2016).
- O. Fialko is an Associate Investigator at the Dodd-Walls Centre for Photonics and Quantum Technologies.
- Sergej Flach is a member of the editorial board of the journal *Chaos: An Interdisciplinary Journal of Nonlinear Science* (American Institute of physics Publishing Journals, impact factor 2.05)
- P. Schwerdtfeger served on the editorial board *Molecular Physics*, *Journal of Computational Chemistry*, *Computational and Theoretical Chemistry*, *Fullerenes, Nanotubes and Carbon Nanostructures* and *Wiley Interdisciplinary Reviews (WIRE): Computational Molecular Science*. He also served several MU boards and committees (including the MU research committee, the Academic Leadership Forum, and the INMS Exec committee). He also met with members of the *International Academy of Quantum Molecular Sciences* to select new fellows (Menton, France, July 2-3). He also served on the selection committee for the Rutherford Medal (Royal Society of New Zealand), and on the Professorial Selection Committee, INMS, Albany.

### *Community Outreach:*

- J.R. Allison helped out at the MU hosted Rotary National Science and Technology Forum and the Metagenomics Workshop, and Massey Open Day.
- P. Bowman spoke to students at the Rotary National Science and Technology Forum.
- J. Brand serves on the organizing committee for the lecture series Fascination Science at Massey University and demonstrated physics experiments at Massey University Open Day.
- E. Pahl started and organized the *Fascination Science* Lecture series at Massey University which was launched with two public lectures in September and October by Profs. Dianne Brunton and Peter Schwerdtfeger which will be continued as a monthly event in 2017. She is member of the INMS Outreach Committee and was involved at the MOTAT Science Street Fair (with a stand with interactive demonstration on *Does it sound wavy? The Physics of Musical Instruments*), organization of the INMS contribution to the STEM and Health Experience Day on 1<sup>st</sup> of June and designed and held a joint physics/chemistry workshop together with Dr. Debbie Jordan on *Hunt for Absolute Zero*, the

physics/chemistry show *Fire and Ice* at Massey Albany Open Day in August and designed and held a Science for Hauora 2016 physics workshop together with Dr Marilou Raduban in October for year 10 and 11 Maori students on *Optical Imaging*. On the 30<sup>th</sup> of July she gave a talk on *Pathways into Natural Sciences* at Kristin School's Tertiary Future Evening.

- P. Schwerdtfeger gave a talk on *Playing with Pentagons and Hexagons – The Wonderful World of Fullerenes* at the Mathematics AGM Meeting, Wellington, February 16; and a public lecture on *Left or Right in Nature – or why is the Universe Left-Handed?* within the Fascination Science Series, Massey University Albany, October 18.
- K.G. Steenbergen led the Science for Hauora 2016 physics workshop, designed to introduce year 11-13 Maori students who are interested in Health Physics to some practical, every-day physics concepts through a physics lab workshop at Massey Albany.

#### *Visits:*

- J.R. Allison visited the group of Prof. Alan Mark, University of Queensland, Brisbane, Australia. She hosted Assist. Prof. Sereina Riniker, ETH Zurich, Switzerland; Dr David Huggins, Cambridge University, UK; Dr Thomas Piggot, Defence Science and Technology Laboratory, UK; Dr Jon Kitchen, University of Southampton, UK; numerous visits from her close collaborator Assoc. Prof. Antony Poole, University of Canterbury, NZ; and the students Dasha Draper, MSc student, Southampton University, UK; Jennifer Crowther, PhD student, University of Canterbury, NZ; Danielle Paterson, PhD student, University of Auckland, NZ; Ali Razzak, MSc student, University of Auckland, NZ.
- J. Brand visited the group of Rodrigo Vicencio at the University of Chile in November 2016 and the group of Ulrich Zuelicke at Victoria University in April and December.
- C. Danieli visited the Center for Theoretical Physics of Complex Systems at the Institute for Basic Science in South Korea between May the 15<sup>th</sup> to July the 30<sup>th</sup>.
- E. Pahl visited the Theoretical Chemistry research group of Prof. L. Cederbaum at the University of Heidelberg, Germany in July.
- P. Schwerdtfeger visited the Theoretical Chemistry Section at the University of Stuttgart, May 2-3.

#### *Exchange Programs:*

- J.R. Allison is part of the University of Southampton MSc student exchange program, hosting MSc students specialising in computational chemistry. She is also part of the A\*STAR Singapore Research Attachment Programme, for co-hosting of PhD students.
- S. Flach is part of the Erasmus Mundus Partnership Program NANOPHOTONICS. The European Commission granted a four-year exchange program NANOPHI on nano photonics (2014-2018) with seven European teams on one side, and an ANU Canberra team and NZIAS on the other side. Its main target is PhD student and postdoc exchange.
- P. Schwerdtfeger, E. Pahl, L. Pašteka and K. Steenbergen are part of a successful grant application entitled *Molecules in Extreme Environments* financed by the Norwegian Academy of Science (total of 3.5 million NOK). It will result in an active exchange program between the University of Oslo and MU. Starting date is 2017.

## Appendix 4

### Financial Statement:

Beside financial support from the College of Sciences through INMS and NZIAS, which covers salaries and administrative support, the following income through internal and external grants was received in 2016 (in NZ\$):

### Grants Received/Continuing:

- J.R. Allison (Fast Start Marsden grant)	100,000
- J.R. Allison (Rutherford Discovery Fellowship)	155,000
- J.R. Allison (AI, Marsden grant)	10,000
- J. Brand (AI on UoO Marsden grant)	38,000
- J. Brand (PI and Theme leader), S. Flach (AI), J. Bodyfelt (AI) and O. Fialko (AI) on CoRE grant of the DWC (2015).	267,769
- O. Fialko (3 <sup>rd</sup> year Marsden FastStart) on “Understanding quantum thermodynamics with the smallest heat engine”	115,000
- O. Fialko (Dodd-Walls Centre New Ideas Research Funding Award)	25,000
- P. Schwerdtfeger and E. Pahl (2 <sup>nd</sup> year Marsden Fund)	250,000

<b>TOTAL</b>	<b>\$ 960,769</b>
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## 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 Pašteka, 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, Mustafa Hassanbulli, Marilou Cadatal-Raduban, Krista Steenbergen, Péter Jeszenszki, Yağmur Kati, Lauri Toikka, Odile Smits, Paul Jerabek, Jan Mewes.*

#### **Personnel:**

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

#### **Secretaries:**

Vesna Davidovic-Alexander (NZIAS)  
Annette Warbrooke (INMS)

## **PhD Students:**

Jayson G. Cosme (Supervisors: J. Brand and O. Fialko)  
William Irvine (Supervisors: J. R. Allison, J.U. Flanagan (UoA) and P. Schwerdtfeger)  
Péter Jeszenszki (Supervisor: J. Brand)  
Yağmur Kati (Supervisors: S. Flach and J. Bodyfelt)  
Elisey Kobzev (Supervisors: J. R. Allison and P. Schwerdtfeger)  
Ashar Malik (Supervisors: J. R. Allison, A.M. Poole and P. Schwerdtfeger)  
Andrew Punnett (Supervisor: P. Bowman)  
Shamim Shadfar (Supervisors: J.R. Allison and T. Fallon)  
Sophie Shamailov (Supervisor: J. Brand)  
Odile Smits (Supervisors: E. Pahl and P. Schwerdtfeger)  
Lukas Trombach (Supervisors: P. Schwerdtfeger and E. Pahl)  
Ivan Welsh (Supervisors: J. R. Allison and P. Schwerdtfeger)

## **BSc(hon)/MSc Students:**

Antony Burrows (Supervisors: E. Pahl and P. Schwerdtfeger)

## **Exchange Students:**

Dasha Draper (University of Southampton)  
Bea von der Esch (LMU Munich).

## **Postdoctoral/Research Fellows:**

Dr Thomas Collier (MU Postdoctoral Fellow)  
Dr. Thomas Engl (Humboldt Feodor-Lynen Fellow)  
Dr. Paul Jerabek (Humboldt Feodor-Lynen Fellow)  
Dr. Jan Mewes (Humboldt Feodor-Lynen Fellow)  
Mrs. Stefanie Mewes (Research Fellow)  
Dr. Lukáš F. Pašteka (MU Postdoctoral Fellow)  
Dr. Krista Steenbergen (Marsden Postdoctoral Fellow)  
Dr. Lauri Toikka (MU Postdoctoral Fellow)

## **Visitors from other institutions:**

### *Long Term:*

Prof. Victor Flambaum (University of New South Wales, Australia) for 1 month in January 2015; Prof. Scott Bohle (Chemistry, McGill University, Canada) for 6 months on sabbatical.

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

Prof. H. Schwarz (TU Berlin, President of the Humboldt Foundation), Prof. Notker Roesch (Technical University of Munich), Prof. Peter Comba (Heidelberg University); Prof. Miroslav Urban, Prof. Stacey Wetmore (University of Lethbridge, Alberta), Prof. Alexander Szameit (Friedrich-Schiller University Jena), Prof. Mahir S. Hussein (University of São Paulo), Prof. Gian-Luca Oppo (University of Strathclyde, Glasgow), Prof. Per Jönsson & Dr. Jörgen Ekman (Group of Material Science and Applied Mathematics, University of Malmö, Sweden), Dr. David Campbell (Department of Physics, Boston University, MA), Prof. Miroslav Urban (Department of Physical and Theoretical Chemistry, Comenius University), Dr. Murray Olson (School of Mathematics and Physics, University of Queensland).