

CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
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2015 MASSEY UNIVERSITY ANNUAL REPORT
CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS



The most dramatic modern revision of Mendeleev's periodic table of elements came in 1944 when Glenn T. Seaborg placed a new series of elements, the actinides (atomic numbers 89–103), below the lanthanides. In this issue of *Nature*, Borschevsky and co-workers report the first measurement of one of the basic atomic properties of element 103 (Lawrencium), namely its first ionization potential.

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 2015), four staff are actively involved in the newly formed Dodd-Walls CoRE, Jane Allison received the prestigious Rutherford Discovery Fellowship, and Joachim Brand received the MU College of Science Research Award. Our articles appear regularly in top international journals (this year for example 2 papers in *Physical Review Letters* and 1 paper in *Nature*. The many high-standing international visitors who joined our research centre in 2015, 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 31 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 started on a new full Marsden grant (Elke Pahl and Peter Schwerdtfeger). Amongst the outstanding achievements were: Jane R. Allison has been awarded the 2015 Rutherford Discovery Fellowships for her research in "Deciphering molecular choreography"; Joachim Brand is the recipient of this years College of Sciences Research Award for his pioneering work on ultracold atomic gases; Sergej Flach was appointed as founding director of the Center of Theoretical Physics of Complex Systems as part of the Institute of Basic Science in Daejeon, South Korea; Peter Schwerdtfeger was the 2015 *Källén Lecturer* at the University of Lund, Physics Department (Sweden), and the *Rutherford Lecturer* in New Zealand; and finally the theoretical chemistry group (P. Schwerdtfeger, E. Pahl, L. F. Pašteka and K. Steenbergen) secured a research contract together with Trgyve Helgaker's group in Oslo for close collaborations on "Molecules in Extreme Environments". Another possible contract with Osaka University is in the making. The large number of international eminent visitors we get each year clearly underlines our international visibility and high level of achievement. Our research centre hosts many international researchers resulting in joint collaborations and publications. For example, MURF funded collaborations with Profs. M. Kaupp (TU Berlin) and D. Sundholm (Helsinki) beginning of 2015 already resulted in published papers in international journals.

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 (Prof. Sergej Flach will move to Korea end of 2016). Moreover, several (probably well-meant) MU policies are not helping to boost research and development in our research centre. On the good news side was a MU grant for our CTCP compute cluster SIMURG received in 2014. The cluster has been upgraded beginning of 2015, and is in operation with more than 1000 cores managed by the Bright Cluster Manager 7.0 + CentOS7 (the cluster is currently 100% in use; for details see

www.massey.ac.nz/~theochem/simurg). For 2016 we intend to further upgrade our compute cluster to retire old nodes (estimated cost ca. 200,000 NZ\$) and to strengthen our activities on Marsden and Dodd-Walls CoRE funded research grants.

Work in progress: There are too many research projects in progress to list all of them (see attachment for more details).

Staffing: 2015 saw a number of additions to our research centre: Yagmur Kati joined as a new PhD student supervised by Sergej Flach. Dr. Paul Jerabek joined the theoretical chemistry group in December this year as an Alexander von Humboldt Feodor-Lynen Fellow (financed by the Humboldt Foundation). And finally, both Mustafa Hassanbuli (Supervisor: P. Schwerdtfeger) and Lukas Wirz (Supervisors: P. Schwerdtfeger and Jane Allison) successfully completed their PhD.

Financial: See Appendix 4.

Acknowledgment: The Director is grateful to all CTCP members for their (again) outstanding performance and very hard work in 2015, and wishes everybody an even more successful year 2016. We enjoyed constant moral and financial support from Profs. Robert Anderson, Ray Geor, Brigid Heywood, Gaven Martin and Allan McBride. 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).



Distinguished Prof. Peter Schwerdtfeger
Director of CTCP, DHOI NZIAS

Date: Thursday, 24 December 2015

Cc: Hon. Steve Maharey (VC), Prof. Gaven Martin (Director, INS and IAS), Prof. Giselle Byrnes (Assistant VC Research, Academic and Enterprise), Prof. Raymond Geor (Pro-VC Science).

Appendix 1

Research and Teaching Objectives for 2016

- 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 Zürich. 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, and an exciting new Bayesian method for extracting structural information from neutron diffraction of disordered materials (with Prof. Andrew Goodwin, University of Oxford), both of which comprise part of the research programme funded by Jane's Rutherford Discovery Fellowship, in addition to his work on enhanced sampling methods (with Deborah Crittenden, University of Canterbury). A third PhD student, Ashar Malik, will continue his work on structural phylogenetics, in particular the development of new metrics for structure comparison, work that is in collaboration with Assist. Prof. Anthony Poole (University of Canterbury) and also comes under the RDF. Finally, 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. Jane will look to continue publishing recent work, and will be hiring a further PhD student and a postdoctoral researcher to enhance the research capabilities of her group, as well as the capacity to develop new and existing collaborative projects, including work on designing inhibitors of protein-protein interactions implicated in cancer with INMS staff member Evelyn Sattler, which was recently awarded Health Research Council funding, potentially game changing research into the true reason for the temperature-dependence of enzyme activity with Prof. Vic Arcus (Waikato University), and work on allosteric plant enzymes with Dr. Ren Dobson (University of Canterbury). Finally, Jane is looking to establish research student exchange programmes with the University of Southampton and A*STAR Singapore.
- J.D. Bodyfelt continues to broaden his research portfolio in the topic of flatband physics in condensed matter. This includes participation in June at the South Korean Institute of Basic Science – Physics of Complex System's "Advanced Study Group: Many Body Localization, Nonergodicity, and All That". In September, Bodyfelt travelled to this year's annual reporting of the Erasmus Mundus' NANOPHI consortium at King's College London, where he also gave an invited colloquium at Northumbria University in Newcastle-Upon-Tyne. This initiated a new project with Arseni Goussev (at Northumbria) on nonlinear dynamics of a Lenz-coupled quantum particle. Lastly, in November he interviewed for an assistant professorship and gave a departmental colloquium at Nazarbayev University, Kazakhstan. Bodyfelt continues to grow his portfolio's topic of lasing nonlinear dynamics: an on-going collaboration with Vassilios Kovanis on line-sharpening of slaved noisy semiconductor lasers will see publication in 2016's first half, tentatively planned to be presented at CLEO and IEEE Photonics West.
- P. Bowman has started a new project (with P. Schwerdtfeger) 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. He is also working on Celestial mechanics simulations for the purpose of demonstrating accretion and tidal forces. The main purpose of this work is pedagogical (although the underlying physics is simple, the consequences can be difficult for students

to grasp), there might also be some research interest due to the simplicity of the approach. Bowman will take over coordination of first year engineering physics in 2016.

- J. Brand will continue to work as a PI on the project “Quantum Emulation and Simulation” funded by the Dodd-Walls Centre of Research Excellence (DWC) with the DWC funded postdoctoral fellows Lauri Toikka and Shreyoshi Gosh in collaboration with CTCP member Oleksandr Fialko. Focus is on the dynamics of quantum vortices and on quantum simulating false vacuum decay models relevant for the physics of the early Universe. In the latter area, a fruitful collaboration with Peter Drummond and Andrei Sidorov of Swinburn University of Technology in Melbourne, Australia will be continued. An additional focus for 2016 is to apply for Marsden funding for a collaboration with Ali Alavi of the Max Planck Institute for Solid State Research in Stuttgart and Martin Zwierlein of MIT. Preliminary work on this project is in progress involving Massey PhD student Peter Jeszinski and MPI postdoctoral fellow Tal Levi. Further work in the Brand research group will continue in the area of quantum features of solitons in one-dimensional quantum gases with Massey PhD candidate Sophie Shamailov. The Marsden-funded project on few-particle dynamics in collaboration with the atom trapping group of Mikkel Anderson of the University of Otago (Brand is AI on the project) is going into an exciting phase in 2016 as experiments are coming into the regime where few-particle quantum dynamics can be probed experimentally. The Brand group is supporting this activity with supporting computer simulations involving Massey PhD candidate Jayson Cosme.
- S. Flach 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 is running for four years and funds extended research visits of PhD students and postdoctoral fellows. Sergej attracted David Campbell at Boston U (USA) who was awarded with a one year Distinguished Visitor Fund of Massey University to deliver a lecture course in March 2016. Sergej will coordinate an ICTP-ECAR international workshop on ‘Disorder, Interactions, Turbulence and Wave Dynamics: Fundamentals and Applications’ in Izmir Turkey in May 2016. The successful series of NZIAS Christmas symposia will be continued with the fourth symposium in 2016 again. Sergej continues to his duty as director of the Center for Theoretical Physics of Complex Systems at the Institute for Basic Science in South Korea. Several CTCP members are scheduled to participate in various international activities there. 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: Work on the Marsden project (together with Peter Schwerdtfeger) will make up the main part of the research in the forthcoming year. Marsden postdoctoral fellow Krista Steenbergen has already joined the group this year and started to work on the development of potential models for the melting of group 12 elements, another postdoctoral student will join in January to work on the melting of molecular systems, and a new PhD student (Odile Smits) will arrive in January to work on rare gas melting under high pressure.

Further collaborations with Prof. Masahiro Ehara (Japan) on catalysis research and Profs Ali Alavi (MPI Stuttgart) and Joachim Brand (CTCP) in the development of a bosonic quantum Monte Carlo code have already started and will be continued. K.G. Steenbergen will continue to work on the melting of Group 12 elements (mercury, zinc and cadmium), extending the existing methods (DIM model) as well as investigating new methods (to include first-principles molecular dynamics). She will begin research on superheavy element 112 (Copernicium), using method of increments to discover the ground state structure. She will continue collaborative work with Osaka University (Prof. Nobuhiko Sarukura and PhD student Luong Viet Mui), simulating the optical properties of crystals of interest for UV laser applications. Elke will teach into physics, coordinating and teaching the first-year Physics for Life Sciences 124.111 paper as well as being involved in second-/third-year teaching within the Physics Minor (Statistical Physics components).

- Boris Pavlov will continue to work on two projects: 1) The resonance mechanism of Earthquakes, and 2) Mathematical modeling of few-dimensional periodic lattices. The first project is in collaboration with V. V. Flambaum (Australia, Sydney) and G. Martin (NZIAS). For 2016 the research plan includes the estimation of the amount of energy transferred from the major tectonic plate to the active zone of the earthquake. Further plans include construction of a fitted solvable model of a tectonic plate with a relatively small active zone attached, with regard of compressure of the active zone defined by the dynamics of neighboring major tectonic plates. The second project is in collaboration with Prof. G. Fursey (St. Petersburg, Russia) and Prof. A. Yafyasov (St. Petersburg, Russia). For 2016 we plan to construct a solvable model of the 2D Metal-carbon interface presented as a periodic 2D superlattice of two lattices with geometrically equivalent periods, with different atomic fillings. Depending on resonance properties of the filling the interface properties may expose various properties scanning from typical metal to semi-conductor or isolator. The intermediate results on the projects will be delivered at a conference in Stockholm, Sweden in mid-March 2016, and at a conference on Applied Mathematics (“Days for Diffraction”) in St. Petersburg, June 2016.
- 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. 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 2016, he is also an invited/plenary speaker at a number of international conferences overseas, and organizer of a conference on the “From Clusters to the Solid State” in Rota, Spain. A number of new PhD students will arrive working on several new topics from cluster modelling to Dirac confinements, and we expect a new postdoctoral fellow to start on phase transitions in January 2016 (together with E. Pahl). 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 2015 refereed journals (members of CTCP are in bold letters):

1. V.M.Adamyan, G. J.Martin and **B. Pavlov**, “Local Scattering problem as a Tool of Perturbation Analysis for Resonance Systems”, *Amer. Math. Soc. Transl.* 233, 1-25 (2014).
2. 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).
3. **A. Borschevsky**, **L. F. Pašteka**, V. Pershina, E. Eliav, U. Kaldor, “Ionization potentials and electron affinities of the superheavy elements 115–117 and their sixth-row homologues Bi, Po, and At”, *Phys. Rev. A* 91, 020501(R)-1-5 (2015).
4. **J. G. Cosme**, **O. Fialko**, “Relaxation dynamics of ultracold bosons in a double-well potential: Thermalization and prethermalization in a nearly integrable model”, *Phys. Rev. A* 92, 033607-1-12 (2015).
5. **C. Danieli**, **J. D. Bodyfelt**, **S. Flach**, “Flat-band engineering of mobility edges”, *Phys. Rev. B* 91, 235134-1-7 (2015).
6. **C. Danieli**, K. Rayanov, **B. Pavlov**, G. Martin, **S. Flach**, “Approximating Metal-Insulator Transitions”, *Int. J. Mod. Phys. B* 29, 1550036-1-13 (2015).
7. M. Ehn, N. Georgiev Vassilev, **L. F. Pašteka**, M. Dangalov, M. Putala, “Atropisomerism of 2,2'-Diaryl-1,1'-binaphthalenes Containing Three Stereogenic Axes: Experimental and Computational Study”, *Eur. J. Org. Chem.* 36, 7935-7942 (2015).
8. **O. Fialko**, B. Opanchuk, A. I. Sidorov, P. D. Drummond, **J. Brand**, “Fate of the false vacuum: Towards realization with ultra-cold atoms”, *Europhys. Lett.* 110, 56001-1-5 (2015).
9. **S. Flach**, **J. D. Bodyfelt**, “Brennpunkt: Eingesperrt - nicht hinter, sondern auf dem Gitter”, *Physik Journal* 14, 24-25 (2015).
10. V. Flambaum, **B. Pavlov**, “A possible resonance mechanism of earthquakes”, *J. Seismol.* 20, 385-392 (2015).
11. G. Fursey, P. Konorov, **B. Pavlov**, A. Yafyasov “Dimensional Quantization and the Resonance Concept of the Low-Threshold Field Emission”, *Electronics* 4, 1101-1108 (2015).
12. D. O. Krimer, **S. Flach**, “Interaction-induced connectivity of disordered two-particle states”, *Phys. Rev. B* 91, 100201-1-5(R) (2015).
13. R. Liao, **O. Fialko**, **J. Brand**, U. Zülicke, “Multicriticality, metastability, and the roton feature in Bose-Einstein condensates with three-dimensional spin-orbit coupling”, *Phys. Rev. A* 92, 043633-1-5 (2015).
14. **A. Munoz Mateo**, **J. Brand**, “Stability and dispersion relations of three-dimensional solitary waves in trapped Bose-Einstein condensates”, *New J. Phys.* 17, 125013-1-18 (2015).
15. **L. F. Pašteka**, **A. Borschevsky**, V. V. Flambaum, **P. Schwerdtfeger**, “Search for variation of fundamental constants: Strong enhancements in $X^2\Pi$ cations of dihalogens and hydrogen halides”, *Phys. Rev. A* 92, 012013-1-9 (2015).

16. K. Rayanov, B. L. Altshuler, Y. G. Rubo, **S. Flach**, “Frequency combs with weakly lasing exciton-polariton condensates”, *Phys. Rev. Lett.* 114, 193901-1-5 (2015).
17. T. K. Sato, M. Asai, **A. Borschevsky**, T. Stora, N. Sato, Y. Kaneya, K. Tsukada, Ch. E. Düllmann, K. Eberhardt, E. Eliav, S. Ichikawa, U. Kaldor, J. V. Kratz, S. Miyashita, Y. Nagame, K. Ooe, A. Osa, D. Renisch, J. Runke, M. Schädel, P. Thörle-Pospiech, A. Toyoshima, N. Trautmann, “Measurement of the first ionization potential of lawrencium, element”, *Nature* 520, 209-211 (2015).
18. **P. Schwerdtfeger**, **L. Wirz**, J. Avery, “The Topology of Fullerenes”, *Wiley Interdisciplinary Reviews (WIRE): Computational Molecular Science* 5, 96-145 (2015). (invited paper).
19. **P. Schwerdtfeger**, **L. F. Pašteka**, **A. Punnett**, **P. Bowman**, “Relativistic and Quantum Electrodynamic Effects in Superheavy Elements”, *Nucl. Phys. A* 944, 551-577 (2015). (invited paper)
20. F. Senn, J. Wiebke, **P. Schwerdtfeger**, **E. Pahl**, “Long-Range Contributions for the Use of Truncated Pair Potentials of Molecular Systems – Application to Nitrogen N₂”, *Mol. Phys.* 113, 1585-1589 (2015).
21. S.-W. Su, S.-C. Gou, I.-K. Liu, A. S. Bradley, **O. Fialko**, **J. Brand**, “Oscillons in coupled Bose-Einstein condensates”, *Phys. Rev. A* 91, 023631-1-8 (2015).
22. D. Sundholm, **L. N. Wirz**, **P. Schwerdtfeger**, “Novel hollow all-carbon structures”, *Nanoscale* 7, 15886-15894 (2015).
23. R. Sure, R. Tonner, **P. Schwerdtfeger**, “A systematic study of rare gas atoms encapsulated in small fullerenes using dispersion corrected density functional theory”, *J. Comput. Chem.* 36, 88-96 (2015).
24. D. K. Theilacker, B. Schlegel, M. Kaupp, **P. Schwerdtfeger**, “Relativistic and Solvation Effects on the Stability of Gold(III) Halides in Aqueous Solution”, *Inorg. Chem.* 54, 9869-9875 (2015).
25. A. Windberger, J. R. Crespo López-Urrutia, H. Bekker, N. S. Oreshkina, J. C. Berengut, V. Bock, **A. Borschevsky**, V. A. Dzuba, E. Eliav, Z. Harman, U. Kaldor, S. Kaul, U. I. Safronova, V. V. Flambaum, C. H. Keitel, P. O. Schmidt, J. Ullrich, O. O. Versolato, “Identification of the Predicted 5s-4f Level Crossing Optical Lines with Applications to Metrology and Searches for the Variation of Fundamental Constants”, *Phys. Rev. Lett.* 114, 150801-1-6 (2015).
26. **L. N. Wirz**, **J. R. Allison**, “Comment on A tensor-free method for the structural and dynamic refinement of proteins using residual dipolar couplings”, *J. Phys. Chem. B* 119, 8223-8224 (2015).
27. **L. N. Wirz**, **J. R. Allison**, “Fitting alignment tensor components to experimental RDCs, CSAs and RQCs”, *J. Biomol. NMR* 62, 25-29 (2015).
28. D. Zare, K. M. McGrath, **J. R. Allison**, “Deciphering β -lactoglobulin interactions at an oil-water interface: a molecular dynamics study”, *Biomacromol.* 16, 1855-1861 (2015).

Refereed Conference Proceedings and arXiv:

29. **J. G. Cosme**, Ch. Weiss, **J. Brand**, “Difficult-to-detect convergence problem of variational multi-mode quantum dynamics with attractive bosons”, 6 pages, arXiv:1510.07845 [quant-ph]

30. L. A. Toikka, J. Brand, "Exactly solvable model for a solitonic vortex in a compressible superfluid", arXiv.

Chapters in Books:

31. S. Flach, "Nonlinear Lattice Waves in Random Potentials ", pp.1-48, in: Springer International Publishing Switzerland 2015 C. Besse, J.-C. Garreau (eds.), Nonlinear Optical and Atomic Systems, Lecture Notes in Mathematics 2146, DOI 10.1007/978-3-319-19015-0_1 .

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=fullerene&menu=fullerenes>



2. Conference and Workshop Presentations

Lectures at Conferences / Meetings:

- J.R. Allison gave keynote lectures at the Molecular Graphics and Modelling Society meeting in Singapore (25-27 November) and the Molecular Modelling 2015 meeting in Sydney (2-5 December) and an invited talk at the Hyam's Protein Research Retreat in Sydney (6-8 December). She gave a selected talk at the NZ Phylogenetics Meeting in Portobello (1-6 February).
- J.D. Bodyfelt gave a contributed talk at IBS Center for Theoretical Physics of Complex Systems' Advanced Study Group: Many Body Localization, Nonergodicity and All That in Daejeon, South Korea, June 23 – July 31; a Massey research reporting for NANOPHI's annual meeting in King's College London September 2-3; a departmental colloquium at Northumbria University's Mathematics department in Newcastle, United Kingdom September 7; and a departmental colloquium for the School of Science & Technology, Nazarbayev University, Kazakhstan, December 1.
- J. Brand gave invited talks at the "2015 Taiwan International Symposium on Contemporary Atomic and Optical Physics" at the Institute of Atomic and Molecular Sciences of the Academia Sinica (Taipei) and the National Center for Theoretical Sciences (NTHU Hsinchu), 8-10 July 2015 in Taiwan; at the "Hybrid Photonics and Materials Conference 2015" in Santorini, Greece 27-31 May 2015; at the Miniconference "Non-equilibrium quantum dynamics in low dimensions" in Durham, UK, 20 – 22 July 2015; at the "Quantum Science Otago Cold Atoms Workshop 2015" in Dunedin 17-18 June 2015. He gave a contributed talk at the "Biennial Conference of the Australian Association of von Humboldt Fellows" in Hobart, Tasmania, Nov 20-22, 2015. J. Brand further delivered a series of three lectures on "Solitons in Quantum Gases" at the Scottish

Universities Summer School “SUSSP71: Frontiers in Quantum Dynamics and Quantum Optics” 21 July to 2 August 2015 at Strathclyde University, Glasgow, UK.

- 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 seven lectures/talks at meetings: invited talk at the 587. WE-Heraeus Seminar “From Photonics to Polaritonics: Non-Equilibrium Transport in Complex Media, Photonic Crystals and Disordered Nano-Structures, April 19-23 2015 in Bad Honnef, Germany; invited lecture at the School on Anomalous Transport, Superconductivity and Magnetism in Nanosystems, June 15-20 2015 in Kyiv, Ukraine; invited talk at the international conference on Nanomechanical Systems: From New Materials to New Applications, July 26-30 2015, Jeju Island, South Korea; invited talk at the conference on Frontiers of Nanoscience, August 24 – September 1 2015, Trieste, Italy; invited talk at the workshop on Violation of Ergodicity, Turbulence and Fractality in Classical and Quantum Dynamical Systems, Sep 21 – Oct 02 2015, Natal, Brazil; invited talk and discussion steering at the program on Many-Body Localization, Oct 12 – Dec 18 2015, Santa Barbara, USA; three invited lectures at the Australian and New Zealand School in Ultracold Physics, Nov 30 – Dec 11 2015, Dunedin, New Zealand.
- E. Pahl gave an invited talk on *Mercury Clusters and the Solid: Challenges of an Ab Initio Description* within the workshop on ‘Theory of metal atoms, clusters and nanoparticles stabilized by organic matter’ held at Aalto University, Helsinki in June and 3 invited talks on *Simulation of Phase Transitions with Highly Accurate Ab Initio Potentials: Applications to Argon, Melting of mercury clusters and the bulk*, and *Search for stable structures in bi-metallic nanoclusters: Application to carbon-halogen bond activation by small gold-palladium clusters* at the 2015 International Chemical Congress of Pacific Basin Societies on (December 15 and 16). Further, she spoke on the AMN-7 in Nelson (February 2015) on *Identification of Stable Structures of Gold-Palladium Bimetallic Nano-Catalysts Based on Density-Functional Theory and Genetic Algorithms: Application to C-Cl Bond Activation in Chlorobenzene* and on the Cluster Meeting 2015 in Whakapapa Village in November on the topic of *Melting under extremely high pressures*.
- B. Pavlov gave two key-note lectures at MCQTN -2015 (Pierre Duclos Workshop), St. Petersburg, Sept. 2015: *The resonance mechanism of Earthquakes* and *Size quantization and the resonance mechanism of Low-Threshold Emission*.
- P. Schwerdtfeger gave a keynote lecture on *Variation of Fundamental Constants in Space-Time* at the Relativistic Satellite Meeting of the International Academy of Quantum Molecular Science in Beijing (June 13). He gave a keynote lecture on “*Variation of Fundamental Constants in Space-Time* at the 14th International Conference Computational and Mathematical Methods in Science and Engineering (CMMSE), Cadiz, Spain (July 7), and a contributed talk on *Golden Dual Fullerenes* at the symposium on “Mathematics meets Chemistry – Theoretical Models at the Nanoscale.” He also gave a talk on *Variation of Fundamental Constants in Space-Time* (July 14) at the 14th Marcel Grossmann “Recent Developments in Theoretical and Experimental General Relativity,

Gravitation, and Relativistic Field Theory” at the University of Rome Sapienza, Rome. He gave plenary lecture on *Playing with Pentagons and Hexagons – From Graphene, to Fullerenes, Fulleroids and Their Golden Duals* at the APPITA Conference on Pulp and Paper in Taupo (August 21); a keynote lecture on *Relativistic Quantum Electrodynamical Effects in Superheavy Elements* at the 34th Mazurian Lakes Conference on Physics (September 11); invited talk at the Biennial Conference of the Australian Association of von Humboldt Fellows: Global Perspectives, Local Knowledge on *Variation of Fundamental Constants in Space-Time*, Hobart, Tasmania (November 21); invited talk at the 2015 International Chemical Congress of Pacific Basin Societies on *Playing with pentagons and hexagons: Fullerenes and their golden duals* (December 19).

- Lauri A. Toikka gave talks on *Vortices and Ring Dark Solitons in Toroidal Bose-Einstein Condensates* at the NZIP Conference 2015, Hamilton; *Dynamics of solitonic vortices*, QSO Cold Atoms Workshop 2015, University of Otago, Dunedin.

Seminars and Talks:

- J.R. Allison gave talks at (i) University of Auckland, Structural Biology group (1 April), (ii) Oxford University, Doctoral Training Centre (27 May), (iii) Oxford University, Department of Theoretical and Physical Chemistry (28 May), (iv) University of Southampton, School of Chemistry (4 June), (v) NIH Bethesda 19 June), (vi) University of Auckland, School of Chemistry (16 September).
- J. Brand gave a talk on “Solitary waves in the strongly-interacting Fermi gas” at the Alavi group seminar at the Max Planck Institute for Solid State Research in Stuttgart, Germany on 16 July 2015. He gave presentations about the research of the Quantum Fluids and Gases Theme of the Dodd-Walls Centre at the DWC Symposium February 2015 in Dunedin and the Scientific Advisory Board meeting 17 November 2015 in Auckland. He gave a 30 minute INMS seminar talk titled “Ernst Chladni’s theory of chimes and three-dimensional solitary waves in atomic superfluids” November 2015 and spoke at Nerd Nite Auckland on “Nonlinear waves in atomic superfluids” in March 2015.
- C. Danieli gave a talk at the Centre for Theoretical Physics of Complex Systems at the Institute for Basic Science in South Korea entitled “Aubry-Andre’ model, approximated and exact MIT” (July 2).
- S. Flach presented four talks: an invited talk at the 2nd IBS-Royal Society colloquium in London, UK; an invited colloquium at the Korean Institute for Advanced Study in Seoul, South Korea; and invited colloquium at the Korean Advanced Institute for Science and Technology in Daejeon, South Korea; a short INMS presentation at Massey University, Albany, New Zealand.
- A. Malik gave a talk at the 19th Annual New Zealand Phylogenetics Meeting in Portobello (3rd February)
- E. Pahl gave a Physics Colloquium talk at University of Auckland on *Melting of Atomic Nano-clusters and Extended Systems: Monte Carlo Simulations with Accurate Interaction Potentials* (October 21) and on *Genetic Algorithm for Nanoclusters: Understanding their Catalytic Activity* within the INMS seminar (October 2).

- P. Schwerdtfeger gave talks at (i) the University of Auckland, Physics Department, on *The End of the Periodic Table – Going for the Superheavy Elements* (March 4), (ii) Victoria University, Chemistry and Physics, on *The Topology of Fullerenes* (March 6), (iii) Osaka University, Laser Physics Section on *High Pressure Physics* (April 14), and in the Chemistry Section on *Relativistic Effects in the Chemistry and Physics of Gold* (April 27), (iv) University of Lund, Physics Department (*Gunnar Källen Lecture Series*): 5 lectures in total on *The Dirac Equation, Variation of Fundamental Constants in Space-Time, Bound-State QED for Heavy Elements, Parity Violation in Chiral Molecules, The End of the Periodic Table – Going for the Superheavy Elements*. (May 18-22); Max-Planck Institute for Solid-State Physics, Stuttgart, on *Variation of Fundamental Constants in Space-Time* (May 26); (v) Universidade de Lisboa (group of Prof. Nico Stollenwerk) on *The Topology of Fullerenes* (June 30); (vi) the Rutherford Public Lecture Series on *Going Superheavy – The End of the Periodic Table* in Hamilton (August 11), Palmerston North (August 13), Wellington (2 lectures August 18 and 19); Christchurch (August 26), Dunedin (August 27) and Auckland (October 7); (vii) University of Otago, Chemistry Department Seminar on *Playing with Pentagons and Hexagons: From Graphene to Graphyne, Fullerenes, Fulleroids, and Gaudienes and their Dual* (August 27); (viii) Center for Multiscale Theory and Computation University at the Westfälische Wilhelms University Münster on *Playing with Hexagons and Pentagons – The Wonderful World of Fullerenes* (October 15); (ix) Kolloquium des Eduard-Zintl-Instituts at the Technische Universität Darmstadt on *Playing with Pentagons and Hexagons: From Graphene to Graphyne, Fullerenes, Fulleroids, and Gaudienes and their Duals* (October 21).
- K.G. Steenbergen gave a talk at the annual New Zealand Cluster Meeting in Whakapapa, Ruapehu titled *The curious case of gallium melting*. She also gave a talk at the 2015 International Chemical Congress of Pacific Basin Societies on *A 2D liquid structure explains the elevated melting temperatures of gallium nanoclusters*.
- Lauri A. Toikka gave talks on *Dark Solitons and Vortices in Quantum Liquids* at the INMS seminar, April 17; *Vortices and Ring Dark Solitons in Toroidal Bose-Einstein Condensates* at the NZIP Conference 2015, Hamilton; *Exactly solvable model for a solitonic vortex in a compressible superfluid*, Physics Seminar, University of Auckland, 18 November 2015; and two internal CTCP seminars.

Poster Presentations:

- J. Brand presented a poster on “Solitary waves in three-dimensional superfluids” at the Aspen Winter Conference, March 23-29, 2015 on “Nonequilibrium Quantum Matter” in Aspen, CO, USA. He also presented posters at the Scientific and Governance Board Meeting of the DWC, 27 November 2015 and the Australian and New Zealand Summer School on Ultracold Atoms, 29 Nov to 11 Dec 2015 in Dunedin.
- Jayson G. Cosme presented posters at the NZIAS-MPIPKS Return Tandem Workshop - Rotorua, New Zealand (2-6 February 2015), and at the 8th Annual Symposium and Launch of the Dodd-Walls Centre - Dunedin, New Zealand (16-17 February 2015).
- C. Danieli presented posters at the NZIAS-MPIPKS Return Tandem Workshop - Rotorua, New Zealand (2-6 February 2015), at the 8th Annual Symposium and Launch of the Dodd-Walls Centre - Dunedin, New Zealand (16-17 February 2015), at the Conference on Frontiers of Nanoscience - Trieste, Italy (August 24 – September 1 2015), at the IONS-KOALA students meeting – Auckland, New Zealand (23-27 November 2015), at the ANZSUP summer school - Dunedin, New Zealand (November 30 – December 11 2015).

- W. Irvine presented a poster titled *A Molecular Dynamics approach to Characterizing the PI3K-Membrane Interaction*, at Molecular Modelling 2015 (MM2015) conference in Sydney organized by the Association of Molecular Modellers of Australasia (AMMA).
- E. Kobzev presented a poster titled *Novel Polarisable Supra-Atomic Phospholipid Models for Multiscale MD Simulations* at MM2015 Conference in Sydney organized by AMMA.
- A. Malik presented a poster titled *Exploring Deep Phylogenies Using Protein Structure*, at MM2015 Conference in Sydney organized by AMMA.
- L. F. Pašteka presented a poster titled *Automated mapping and computation of the complete rearrangement networks of substituted bullvalene* at the 15th International Congress of Quantum Chemistry 2015 in Beijing, China (8-13 June). He also presented a poster titled *Search for variation of fundamental constants: Strong enhancements in $X^2\Pi$ cations of dihalogens and hydrogen halides* at the ICQC satellite meeting New Frontiers of Relativistic Quantum Chemistry 2015 in Beijing, China (13-16 June). He also presented two posters on these topics at the 2015 International Chemical Congress of Pacific Basin Societies in Honolulu HI, USA (15-20 December).
- S. S. Shamailov presented a poster at the ANZSUP summer school in Dunedin, New Zealand (30/11/2015-11/12/2015).
- Lauri A. Toikka presented posters on *Exactly solvable model for a solitonic vortex in a compressible superfluid*, IONS KOALA, University of Auckland, November 27 2015; and on the same topic at ANZSUP 2015, University of Otago, December 9 2015.
- I. Welsh presented a poster titled *Magical Cherries: Automated Parameterisation of the World* at MM2015 Conference in Sydney organized by AMMA.

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
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 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

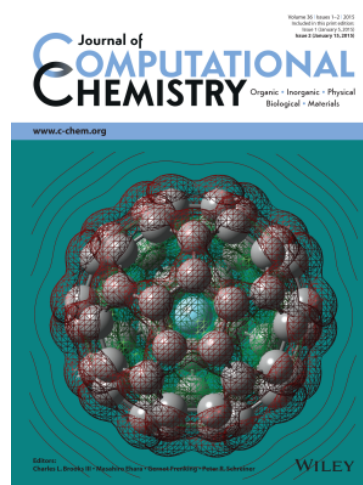
2. PROFESSIONAL LEADERSHIP AND ADMINISTRATION

Honours and Awards:

- J.R. Allison has been awarded the 2015 Rutherford Discovery Fellowships for her research in "Deciphering molecular choreography". The Fellowships foster the development of future research leaders by providing funding of up to \$800,000 over five years to cover salary and research costs.
- Joachim Brand is the recipient of this years College of Sciences Research Award for his pioneering work on ultracold atomic gases.
- Dr. Mustafa Hasanbulli successfully completed his second PhD degree and may now call himself Dr. Dr. or Dr. square. He investigated in detail physical properties of various atomic systems such as hydrogen, helium and argon confined in a soft-wall potential.
- L. F. Pašteka received a poster award for a poster titled *Automated mapping and computation of the complete rearrangement networks of substituted bullvalene* presented at the 15th International Congress of Quantum Chemistry 2015 in Beijing, China (8-13 June).
- P.Schwerdtfeger was the Gunnar Källén Lecturer of 2015 at the University of Lund, Department of Physics, and the 2015 New Zealand Rutherford Lecturer.

Publicity:

- A. Borschevsky's work [see *Nature* **520**, 209 (2015)] on the measured ionization potential for the exotic element with nuclear charge 103 made it into the international news, see for example D. Castelvechi, "Exotic atom struggles to find its place in the periodic table", *Nature* April 8 issue (2015), or ScienceDaily at www.sciencedaily.com/releases/2015/04/150409081434.htm.
- P. Schwerdtfeger et al. had a title page awarded by the *Journal of Computational Chemistry* **36**, 88-96 (2015). (picture on the left). Encapsulating rare-gas atoms into fullerenes smaller than C₆₀ quickly becomes repulsive and follows an exponential law with decreasing number of carbon atoms. The reason comes from a rather rigid cage structure that determines the space available inside the fullerene. His work on gaudienes in collaboration with Dage Sundholm from the University of Helsinki went into the ChemistryWorld News: Molecular legacy of Antoni Gaudi (see <http://www.rsc.org/chemistryworld/2015/09/molecular-legacy-gaudi-carbon-cage>).



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): *Many-body interactions in quasi-periodic potentials*. (Supervisors: S. Flach, G. Martin, J. Bodyfelt).
- Yağmur Kati (first year): *Space-Time Correlations for Nonergodic Disordered Nonlinear Waves*.
- Andrew Punnett (sixth year): *How Hadrons keep their Quarks*. (Supervisor: P. Bowman).
- Sophie Shamailov (third 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)
- Ashar Malik (second year): *The evolution of phylogenetics: from sequence to structure*. (Supervisors: J.R. Allison, A.M. Poole (U. Canterbury) and P. Schwerdtfeger).
- William Irvine (second 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.
- Elisey Kobzev (second year): *Development and application of multiscale models for biomolecular simulation*. (Supervisors: J.R. Allison and P. Schwerdtfeger).
- Ivan Welsh (second year): *Automated parameterisation of the world**. (Supervisors: J.R. Allison and P. Schwerdtfeger)

Finished PhD Theses:

- Lukas Wirz (third year): *Computer Modelling of Fullerenes / Biasing molecular modelling with experimental RDCs*. (Supervisors: P. Schwerdtfeger and J.R. Allison).

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 124.129 (Astronomy) and 124.350 (Computational Physics); taught into 246.102 (Core Skills for Natural Scientists) and 246.302 (Research Themes in Natural Sciences) and delivered special lectures for high performing first-year physics students.
- 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 first half of this paper. She also taught the 3-weeks module on *Monte Carlo Integration* in the third-year 124.350 *Computational Physics* paper, 4 weeks into the 124.102 *Physics* paper and supervised a 124.129 *Astronomy* lab.

- 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), and 9 lectures on *Chemical Evolution Theory* for the *Research Themes in Natural Sciences* paper 246.302 (semester 2).
- K.G. Steenbergen gave lecture courses (16 lectures) for the paper 124.100.

Other activities:

Papers refereed:

- J.R. Allison refereed papers for the journals *Journal of Chemical Theory and Computation*, *Journal of Molecular Graphics and Modeling*, *Nature Scientific Reports*, *PhysChemChemPhys* and *Structure*.
- J. Bodyfelt refereed papers for *IEEE Journal of Selected Topics in Quantum Electronics*, *Physical Review E*, *Philosophical Transactions A*, *International Journal of Modern Physics B*, and *Journal of Physics A*.
- J. Brand refereed papers for *Nature Physics*, *New Journal of Physics*, *Physical Review Letters*, *Physical Review A*, and *Fortschritte der Physik – Progress in Physics*.
- S. Flach refereed paper for several physics journals.
- E. Pahl refereed papers for *Journal of the American Society*, *Journal of Physical Chemistry*, *Chemical Physics Letters*, *Chemical Physics D*, *New Journal of Physics*, *Physical Chemistry Chemical Physics*, and *Journal of Computational Chemistry*.
- P. Schwerdtfeger refereed in total 62 papers (rejecting about 2/3 of the invitations) from 32 different international journals including *Angewandte Chemie*, *Nature*, *Physical Review Letters* and *J. Am. Chem. Soc.*
- K.G. Steenbergen refereed 2 papers in total.
- L. A. Toikka refereed in total 7 manuscripts for *Phys, Rev. A*, *Phys, Rev. E*, *New J. Phys.*, *J. Phys. B*.

PhD/MSc and other theses refereed:

- J.R. Allison examined PhD theses from the University of Queensland (group of Alan Mark) and Massey University (group of Paul Rainey), an MSc thesis from the University of Canterbury (group of Renwick Dobson) and a PGDipSci thesis from the University of Auckland (group of Johannes Reynisson).
- P. Bowman examined a MSc thesis from Auckland University and a PhD thesis from Massey University.
- J. Brand examined a PhD thesis in Physics at Victoria University of Wellington as referee and oral examiner.
- E.Pahl refereed a PhD thesis from Zhi Xiang Wong (group of Matthias Lein at Victoria University Wellington) with the oral examination in Wellington on 19th February. She also was examiner in the PhD confirmations of Elisey Kobazev and Ivan Welsh from group of Jane Allison.
- P. Schwerdtfeger refereed a PhD thesis from Victoria University Wellington (group of Prof. U. Zülicke). The oral examination took place in Wellington March 6.

Graduate Summer School Organisation:

- J. Brand organised (as chair of the organising committee) the Australian and New Zealand Summer School in Ultracold Physics (ANZSUP 2015) in Dunedin, 29 Nov to 11 Dec 2015. With more than 40 graduate students from eight countries and high calibre international lecturers (including Nobel laureate W.D. Phillips from NIST, USA) the graduate school organised through the Dodd-Walls Centre was a great success.

Conference Organisation:

- J.R. Allison organised the highly successful Proteins satellite meeting at Queenstown Research Week (3-4 September), and is again on the organising committee of the main Queenstown Molecular Biology meeting for 2016.
- S. Flach and J. Brand organized the second NZIAS-MPIPKS Tandem Workshop 2015 on Physics of Complex Systems. This return part of the Exploratory Tandem Workshop Event was run jointly by the New Zealand Institute for Advanced Study (Auckland, New Zealand) and the Max Planck Institute for the Physics of Complex Systems (Dresden, Germany). Its focus was on applying stochastic methods to the complex dynamics of nanoscale, mesoscale, and macroscale systems. Prospective topics included stochastic field approaches to quantum many-body physics, quantum noise in interferometry, quantum dissipative condensates, many-body localization, and dynamics of noisy non-equilibrium quantum many-body systems. The meeting was held at the beautiful lakeside resort of Novotel Rotorua Lakeside in New Zealand, February 2-6, 2015.
- P. Schwerdtfeger was part of the organizing committee for the 14th International Conference Computational and Mathematical Methods in Science and Engineering CMMSE), Cadiz, Spain (July 6-10) and ran a symposium (together with Ottorino Ori and Ian Hamilton) on “Mathematics meets Chemistry – Theoretical Models at the Nanoscale.” He is also on the organizing committee of four different symposia at the The International Chemical Congress of Pacific Basin Societies 2015, held in Honolulu (December 15-20).

Conference Participation:

- J.R. Allison attended the Gordon Research Conferences on Computational Aspects of Biomolecular NMR in Italy (7-12 June) and on Proteins in New Hampshire (14-19 June).
- P. Schwerdtfeger attended the 2015 IAQMS conference in Beijing (June 8-13) and attended the IAQMS board meeting (June 7), and the Inorganic Chemistry Symposium in Münster, Germany, in honour of Prof. Ekkehardt Hahn (October 16).

Chairs at Conferences:

- J.R. Allison chaired sessions at the Proteins satellite meeting at Queenstown Research Week (3-4 September) and the session on Biomolecular Simulation at the Molecular Modelling 2015 meeting in Sydney (2-5 December).
- J. Brand chaired sessions at the JQI mini conference in Durham, UK and that the Taiwan Symposium for Contemporary Atomic Physics.
- E. Pahl chaired two sessions at the workshop on “Theory of metal atoms, clusters and nanoparticles stabilized by organic matter” in Helsinki, Finland.
- P. Schwerdtfeger chaired the opening session of the 14th International Conference Computational and Mathematical Methods in Science and Engineering CMMSE), Cadiz, Spain (July 6-10) and the opening session of the symposium on “Mathematics meets Chemistry – Theoretical Models at the Nanoscale” at that conference. He also chaired 3

sessions at different symposia on “Theory of Main Group Chemistry Beyond First Row”, International Chemical Congress of Pacific Basin Societies 2015, Honolulu (December 16), the symposium on “Synergistic Relationships between Computational Chemistry and Experiment” (December 19), and at the symposium on “The Expanding Periodic Table: New Discoveries and Chemistry of the Heaviest Elements” (December 20).

Boards / Editorial Boards / Professional Societies / Memberships:

- J.R. Allison was elected a member of the RSNZ Early Career Researcher committee that has established an ECR sub-membership of RSNZ. She is also the NZ representative on the committees of the Australasian Biophysics Society and the Association of Molecular Modellers of Australasia.
- 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.
- O. Fialko is an Associate Investigator at the Dodd-Walls Centre for Photonics and Quantum Technologies.
- 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).

Community Outreach:

- J.R. Allison helped at the Massey University section of the nationwide Metagenomics day, spoke at the Massey University hosted Biology Olympic training camp, and helped at the Massey University Auckland Open Day.
- P. Bowman spoke to high school students at the Rotary Science Forum, January 13th-15th.
- J. Brand spoke at Nerd Nite Auckland on “Solitary Waves in Atomic Superfluids”, March 2015.
- E. Pahl organized and attended the physics stand “Does it sound Wavy?” on the Physics behind musical instruments at Motat on March 29th. She also was involved in the planning and performance of the Chemistry and Physics Show at the Massey University Open Day. She coordinated the INMS contributions to the Sci/Tech/Health/Eng Experience Day on 4th of June. She is member of the INMS Outreach Committee.
- P. Schwerdtfeger attended a German – New Zealand Business Meeting in Wellington by invitation of the German Embassy (June 3); He gave a lecture at the U3A (University of the 3rd Age) in Auckland on “Playing with Pentagons and Hexagons – The Wonderful World of Fullerenes (October 27), and at the same day was the guest speaker at the Diocesan Music and Arts Awards 2015 Event, Diocesan School for Girls giving a speech on *The value of music and arts in our education* (see picture on the right swapping his science tie for an art tie).
- L. A. Toikka, K. G. Steenbergen, E. Pahl and J. Brand participated at Massey Open Day (physics demonstrations).



Visits:

- J.R. Allison visited the groups of Assist. Prof. Sereina Riniker (ETH Zurich), Assoc. Prof. Anthony Poole (University of Canterbury), Prof. Andrew Goodwin (Oxford University), Assist. Prof. Lorna Smith (Oxford University), Prof. Jon Essex (University of Southampton) and Rob Best (NIH Bethesda).
- J. J. Bodyfelt visited the groups of Anatoly Zayats (King's College London), Arseni Goussev (Northumbria University), Vassilios Kovanis (Nazarbayev University), and Anton Desyatnikov (Nazarbayev University).
- J. Brand visited the group of Ali Alvi at the Max Planck insitute for Solid State Research in Stuttgart, Germany in July 2015 to initiate a collaboration and discuss a Marsden proposal.
- C. Danieli visited the Center for Theoretical Physics of Complex Systems at the Institute for Basic Science in South Korea between July and August.
- O. Fialko was a visiting researcher at the Fujian Normal University, China, funded by Fujian Normal University.
- Peter Jeszinszki visited the group of Ali Alvi at the Max Planck insitute for Solid State Research in Stuttgart, Germany in October and November 2015 to work on a research project in collaboration with Joachim Brand, Ali Alavi and Tal Levi.
- E. Pahl visited the research group in Theoretical Chemistry of Prof. L. Cederbaum at the University of Heidelberg in June.
- P. Schwerdtfeger spent one month at Osaka University at the Osaka 2 Petawatt Laser Facility (March 30-May 2) for future collaborations on optical properties of solid-state materials (research group of Prof. N. Sarukura). Osaka's powerful laser is called [LFEX](#), or Laser for Fast Ignition Experiments, and measures more than 300 feet long. The visit resulted in an active exchange program between both groups. He also visited the Centro de Matemática, Aplicações Fundamentais e Investigação Operacional, Faculdade de Ciências da Universidade de Lisboa (group of Prof. Nico Stollenwerk, June 25 – July 3). He also visited the University of Stuttgart and the Max-Planck Institute in Stuttgart on a regular basis.

Exchange Programs:

- 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 2018.
- 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.

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 2015 (in NZ\$):

Grants Received/Continuing:

- J. Allison (Fast Start Marsden grant)	100,000
- J. Allison (Rutherford Discovery Fellowship)	155,000
- 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 rd 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
- E. Pahl (MURF Visitor funding)	2,700
- P. Schwerdtfeger (MURF Visitor funding)	1,000
- P. Schwerdtfeger and E. Pahl (1 st year Marsden Fund)	250,000

TOTAL **\$ 954,469**

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 Shamailov, 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 Hassanbuli, Marilou Cadatal-Raduban, Krista Steenbergen, Péter Jeszenszki, Yağmur Kati, Lauri Toikka.

Personnel:

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

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

Prof. Sergej Flach (Physics)

Prof. Boris Pavlov (Mathematical Physics)

Dr. Jane Allison (Senior Lecturer, Biological Sciences)

Dr. Elke Pahl (Senior Lecturer, Physics)

Dr. Patrick Bowman (Senior Lecturer, Physics)

Dr. Joshua Bodyfelt (Research Officer)

Dr. Oleksandr Fialko (Marsden fellow)

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

Honorary CTCP Members:

Dr. Anastasia Borschevsky (University of Mainz)

Secretaries:

Vesna Davidovic-Alexander (IAS)

Coleen van Es (INMS)

PhD Students:

Jayson G. Cosme (Supervisors: J. Brand and O. Fialko)
Mustafa Hasanbulli (Supervisor: P. Schwerdtfeger)
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)
Sophie Shamilov (Supervisor: J. Brand)
Lukas Trombach (Supervisors: P. Schwerdtfeger and E. Pahl)
Ivan Welsh (Supervisors: J. R. Allison and P. Schwerdtfeger)
Lukas Wirz (Supervisors: P. Schwerdtfeger and J. R. Allison)

MSc Students:

none

Exchange Students:

Mr. Luong Viet Mui (Osaka University).

Postdoctoral/Research Fellows:

Dr. Lukáš F. Pašteka (MU Postdoctoral Fellow)
Dr. Paul Jerabek (Humboldt Feodor-Lynen 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, 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. Other long-term visitors (sabbatical): Prof. Martin Kaupp (TU Berlin; Jan 1 – Feb 28), AProf. Kelling Donald (Richmond University, USA; Jan 5 – Apr 4), Prof. Dage Sundholm (University of Helsinki; Jan 19 – March 20), Prof. Andrei Derevianko (January 3-31) and Prof. Phil Bunker (National Research Council, Ottawa, Canada, November).

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

Dr. Nicola Gaston (U Victoria), Prof. Beate Paulus, Prof. Yun Li (ANU Canberra), Prof. Nobuhiko Sarukura (Osaka University), Dr. Alex Ayet (Ecole normale superieure, France), Dr. Andrew Hilliard (Institute for Physics and Astronomy, Aarhus University, Denmark), Dr. Elena Mena-Osteritz (University of Ulm, Organic Chemistry), Dr. Andreas Stegmüller (Philipps University Marburg).