

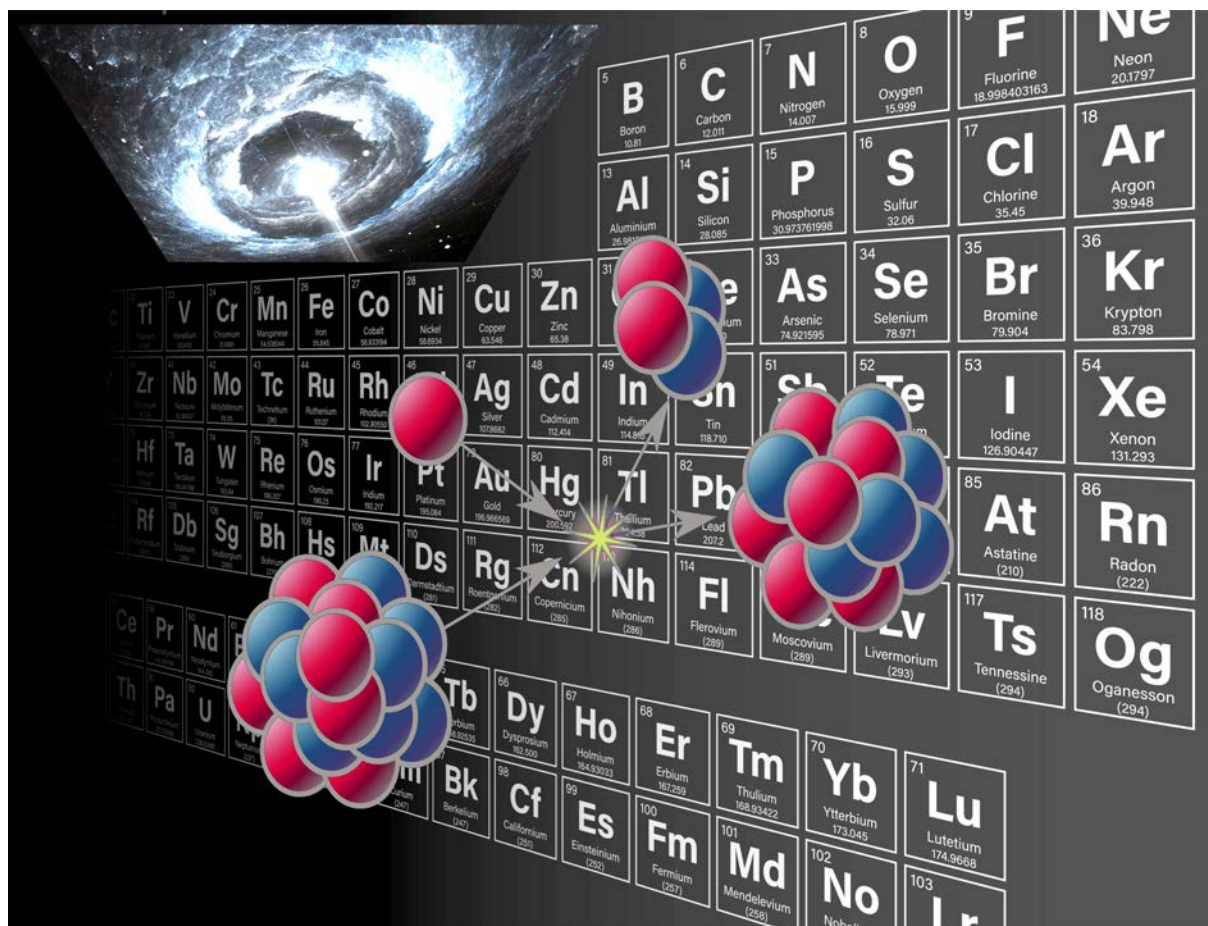
**CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS (CTCP)
NEW ZEALAND INSTITUTE FOR ADVANCED STUDY (NZIAS),
INSTITUTE OF NATURAL AND MATHEMATICAL SCIENCES (INMS)**

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**2020 MASSEY UNIVERSITY ANNUAL REPORT
CENTRE FOR THEORETICAL CHEMISTRY AND PHYSICS**



The periodic table and the physics that drives it. As the International Year of the Periodic Table came to an end in 2019, we reflect on the chemistry and physics that drive the periodic table of the elements. This includes aspects of periodic trends, relativistic electronic-structure theory, nuclear-structure theory and the astrophysical origin of the elements.

Nature Review Chemistry **4**, 359-380 (2020)

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

All objectives are clearly met. We are one of the most productive and internationally acclaimed theoretical research centres 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 in 2004. Joachim Brand is actively involved in the Dodd-Walls CoRE for Photonics and Quantum Technologies and the Max-Planck Institute of Solid State Physics in Stuttgart, Marilou Raduban is a member of the Institute of Laser Engineering at Osaka University, and Peter Schwerdtfeger has strong engagements with Michigan State University in the US and the Laboratoire Kastler Brossel in Paris, France. There were many visits planned to conferences and universities, but 2020 was the year of Covid-19 with travel restrictions imposed severely affecting our research performance.

Research Output: This year we published 22 papers in international journals.

Activities and achievements: All members of CTCP were actively involved in chemistry and physics teaching as outlined in Appendix 4.

The Future - Opportunities, Risks and Directions: We are (and continue to be) a top research centre of international high standing. This is achieved despite the fact that very limited financial resources are available and little moral support coming from MU. Unnecessary bureaucratic hurdles and policies are put into place making academic life very difficult, especially for those working in fundamental sciences. The risks are very clear: Other universities overseas are far better resourced. We have already experienced the loss of excellent staff, end in 2020 even more so with the threat to close down a very successful school (School of Natural and Computational Sciences) at the Albany Campus. Yet we are contributing enormously to the international reputation and ranking of Massey University and therefore deserve far better recognition.

Work in progress: See attachment for more details.

Financial: See Appendix 5.

Acknowledgment: The Director is grateful to the few remaining CTCP members for their outstanding performance and very hard work in 2020, and he wishes everybody an even more successful and productive year 2021 despite the enormous financial pressure imposed upon the College of Science and our Institute, and the travel restrictions due to Covid-19. My very special thanks go to our Institute's secretary, Mrs Vesna Davidovic-Alexander (IAS), who has helped us so much to run our research centre efficiently, organizing conferences and meetings, looking after our overseas visitors, and relocating the NZIAS to the new premises. We acknowledge on-going support by the Pro-VC Prof. Ray Geor as well as Liz Thaisen (for financial advice). We are also very grateful to Mike Yap for his excellent support in terms of system administration on our compute cluster.



Distinguished Prof. Peter Schwerdtfeger
Director of CTCP, HOI NZIAS
Date: Tuesday, 31 March 2021

Appendix 1

Research and Teaching Objectives for 2021

- J. Brand continues work on his Marsden project “Playing dice with Fermi: Full configuration interaction quantum Monte Carlo for fermionic atoms” and on his project “Artificial gauge fields and topological excitations” in the Dodd-Walls Centre for Photonic and Quantum Technologies. He is currently supervising two PhD students (Mingrui Yang and Sarthak Choudhury) and three postdoctoral fellows (Ulrich Ebling, Peter Jeszenski, and Jan Major). Objectives for 2021 are to conclude the previous Marsden project and start work on the new Marsden project “Three atoms in a tight spot”. Dodd-Walls Centre funding has also been renewed and a new project led by JB is starting with the title “Topological materials and coupled superfluids”.
- M. Raduban will continue her work on the numerical investigation of wide band gap fluoride crystals as laser materials in the short wavelength vacuum ultraviolet region, funded by MURF. She will start a new project funded by SREF on the numerical and experimental investigation of wide band gap fluoride crystals as scintillators especially under high pressure conditions. The experimental aspect of this SREF project will be done in collaboration with the Institute of Laser Engineering, Osaka University, consequently strengthening the partnership between Massey University and Osaka University. She is scheduled to travel to Osaka University as a visiting Assistant Professor from January to March. The trip will be fully funded by Osaka University. M. Raduban also plans to start a new collaboration with Dr. Jiri Olejníček from the Institute of Physics, Academy of Sciences of the Czech Republic in Prague, Czech Republic as she explores a new research area of high energy radiation detection using thin film photoconductive detectors. She is scheduled to travel to Prague in March to initiate the collaboration. In terms of teaching, M. Raduban will coordinate and teach into the Auckland offering of 124.103 Biophysical Principles in semester 1. She will also teach into 124.105 Physics 1B in semester 2.
- P. Schwerdtfeger will continue his work on the current Marsden grant (Going Superheavy - Exploring the Chemistry and Physics of the Heaviest Elements in the Remotest Corner of the Periodic Table) and Dumont d’Urville grant (Predicting the correct ground states for superheavy elements beyond nuclear charge 120). We continue with the many research topics in our group which currently involves four PhD students and one postdoctoral fellow. Several collaborations are anticipated with research groups from overseas (Profs. P. Indelicato and T. Saue, France, Drs. P. Jerabek and J. Mewes, Germany, and Prof. W. Nazarewicz in the US), and participation at a number of online conferences have already been agreed on as an invited speaker. I will continue my work on the MU Academic Board representing academic staff within the CoS, the International Academy of Quantum Molecular Sciences to elect new members, and teaching chemistry courses at year 2 and 3. I am part of two proposals currently pending, an ERC Advanced Grant project HAMP-VQED (Highly Accurate Molecular Properties using variational Quantum Electrodynamics), and an MBIE proposal (NZ-German Green H₂ alliance: delivering 100%).

Appendix 2

1. Research Output, Publications and Reports

Articles published in 2020 refereed journals (2020 members of MU are in bold letters):

1. **A. Burrows, S. Cooper, E. Pahl, P. Schwerdtfeger**, “Analytical methods for fast converging lattice sums for cubic and hexagonal close-packed structures”, *Journal of Mathematical Physics* 61, 123503-1-35 (2020). (dedicated to J. Zucker for his 88th birthday)
2. **M. Cadatal-Raduban**, A. Yoshikawa, L. V. Mui, M. H. Pham, T. Shimizu, N. Sarukura, T. Togashi, K. Yamanoi, “Investigation of cross luminescence in lanthanum fluoride as a potential fast-response scintillator”, *Japanese Journal of Applied Physics* 59, 052005 (2020).
3. T. B. Nguyen, T. B. Vu, D. C. Nguyen, T. T. Do, H. M. Pham, **M. Cadatal-Raduban**, “Photodynamic Properties of CdSe/CdS Quantum Dots in Intracellular Media”, *Applied Sciences* 10, 3988 (2020).
4. **P. Jeszenszki, U. Ebling**, H. Luo, A. Alavi, **J. Brand**, “Eliminating the wave-function singularity for ultracold atoms by a similarity transformation”, *Physical Review Research* 2, 043270-1-14 (2020).
5. Y. Lai, H. Yu, T. Ishimoto, **M. Cadatal-Raduban**, S. Kothan, P. Limkitjaroenporn, T. Shimizu, N. Sarukura, J. Kaewkhao, K. Yamanoi, “Investigation of gamma-ray induced optical property changes in non-doped and Ce-doped lithium-rich oxide glass”, *Radiation Physics and Chemistry* 179, 109272 (2020).
6. M. V. Luong, N. Sarukura, M. H. Pham, **P. Schwerdtfeger, M. Cadatal-Raduban**, “Numerical investigation of the electronic and optical properties of LiLuF₄ vacuum ultraviolet material”, *Japanese Journal of Applied Physics* 59, 072001-1-6 (2020).
7. Y. Minami, **M. Cadatal-Raduban**, K. Kuroda, K. Shinohara, Y. Lai, K. Yamanoi, N. Sarukura, T. Shimizu, R. Ishii, Y. Kawakami, N. Kabasawa, T. Amano, K. Kiyohara, M. Kiyohara, “Achromatic Deep Ultraviolet Lens Using Novel Optical Materials”, *Physica Status Solidi b* 257, 1900480 (2020).
8. M. V. Luong, N. Sarukura, M. H. Pham, **P. Schwerdtfeger, M. Cadatal-Raduban**, “Numerical investigation of the electronic and optical properties of LiLuF₄ vacuum ultraviolet material”, *Japanese Journal of Applied Physics* 59, 072001-1-6 (2020).
9. J. M. Mewes, **O. R. Smits**, “Accurate elemental boiling points from first principles”, *Physical Chemistry Chemical Physics* 22, 24041-24050 (2020).
10. **A. J. Nielson, J. Harrison**, A. Sajjad, **P. Schwerdtfeger**, “Electronic and Steric Manipulation of the Agostic Interaction in benzo[h]quinolone Complexes of Pd(II) and Implications for the Formation of η^1 -Pd–C Bonds”, *European Journal of Inorganic Chemistry* 27, 2639-2650 (2020).
11. **A. J. Nielson**, M. A. Sajjad, **P. Schwerdtfeger, J. Harrison**, “A Search by NBO Analysis for Syndetic Donation in Known X-ray Structures of Transition Metal Complexes with Close Aromatic Ring C–H \cdots Metal Approaches”, *European Journal of Inorganic Chemistry* 27, 2603-2614 (2020).

12. B. D. Ostojić, **P. Schwerdtfeger**, A. Nakayama, J. Hasegawa, D. S. Đorđević, “A detailed analysis of the spin-crossover reaction of H₂S binding to heme and the six-coordinated FeP(Im)-HS- porphyrin complex”, *Journal of Inorganic Biochemistry* **206**, 111049-1-11 (2020).
13. L. F. Pasteka, T. Helgaker, T. Saue, D. Sundholm, H.-J. Werner, M. Hasanbuli, J. Major, **P. Schwerdtfeger**, “Atoms and molecules in soft confinement potentials”, *Molecular Physics* **118**, e1730989-1-23 (2020). (dedicated to Jürgen Gauss for his 60th birthday)
14. L. A. Reynolds, E. Schwartz, **U. Ebling**, M. Weyland, **J. Brand**, M. F. Andersen, “Direct measurements of collisional dynamics in cold atom triads”, *Physical Review Letters* **124**, 073401-1-7 (2020).
15. **O. Smits**, J.-M. Mewes, P. Jerabek, **P. Schwerdtfeger**, “Oganesson - A noble gas element that is neither noble nor a gas”, *Angewandte Chemie International Edition* **59**, 23636-23640 (2020); *Angewandte Chemie* **132**, 23843-23848 (2020).
16. O. Smits, P. Jerabek, **E. Pahl**, **P. Schwerdtfeger**, “First principles melting of krypton and xenon based on many-body relativistic coupled-cluster interaction potentials”, *Physical Review B* **101**, 104103-1-12 (2020).
17. **P. Schwerdtfeger**, **O. Smits**, P. Pykkö, “The Periodic Table and the Physics That Drives It”, *Nature Review Chemistry* **4**, 359-380 (2020). (invited paper, dedicated to H.W. Kutzelnigg in memoriam)
18. K. Thompson, **J. Brand**, U. Zülicke, “Chiral two-dimensional wave superfluid from wave pairing in the Bose-Einstein-condensate regime”, *Physical Review A* **101**, 013613-1-11 (2020).
19. M. Yang, **E. Pahl**, **J. Brand**, “Improved walker population control for full configuration interaction quantum Monte Carlo”, *The Journal of Chemical Physics* **153**, 174103-1-14 (2020).
20. K. Yamanoi, Y. Minami, T. Shimizu, N. Sarukura, T. Murata, H. Yoshida, S. Fujino, **M. Cadatal-Raduban**, “Luminescence Properties of Nd³⁺-Doped AlF₃-Based Fluoride Glass in the Vacuum Ultraviolet Region”, *Physica Status Solidi b* **257**, 1900475 (2020).
21. X. Yu, **M. Cadatal-Raduban**, S. Kato, M. Kase, S. Ono, “Femtosecond PLD-grown YF₃ nanoparticle thin films as improved filterless VUV photoconductive detectors”, *Nanotechnology* **32**, 015501 (2020).
22. X. Yu, S. Kato, H. Ito, S. Ono, M. Kase, **M. Cadatal-Raduban**, “Filterless tunable photoconductive ultraviolet radiation detector using CeF₃ thin films grown by pulsed laser deposition”, *AIP Advances* **10**, 045309 (2020).

Refereed Conference Proceedings and arXiv:

NA

Chapters in Books:

NA

Software developments:

J. Brand, E. Pahl, M. Yang: Rimu.jl: An open-source Julia program to calculate ground state properties of bosonic systems with FCIQMC. Published at <https://github.com/joachimbrand/Rimu.jl>

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

P. Schwerdtfeger: Program SAMBA: A Fortran program to calculate solid-state properties through many-body expansions.

P. Schwerdtfeger, A. Burrows, S. Cooper: Program *Jones*: A Fortran program to calculate lattice sums for cubic and hexagonal closed packed lattices.

M. Piibeht, L. F. Pašteka: Contributions to the development of *GRASP*, the General Relativistic Atomic Structure Package (<https://github.com/compas/grasp>), as part of the CompAS collaboration.

M. Piibeht: Contributions to the HelFEM finite element library (<https://github.com/susilehtola/HelFEM>), the related Julia wrapper (<https://github.com/mortenpi/HelFEM.jl>) and to the JuliaAtoms GitHub organization (<https://github.com/JuliaAtoms>) containing various Julia packages for atomic physics and quantum chemistry calculations.



2. Conference and Workshop Presentations

Lectures at Conferences / Meetings / Workshops:

- M. Raduban gave an invited talk on *Filterless vacuum ultraviolet photoconductive detector based on compound fluorides with controllable band gap* at the 9th Global Conference on Materials Science and Engineering in Ukraine (virtual, November 20-23). She also gave an invited talk on *Fast-response scintillation through cross luminescence in wide band gap fluoride crystals* at the 5th International Conference on Smart Materials and Nanotechnology in Thailand which was held in hybrid mode where participants from Thailand attended face-to-face while overseas participants joined via Zoom (December 1-4).
- P. Schwerdtfeger gave an invited talk on *From sticky hard spheres to Lennard-Jones potentials and rare gas solids* at the Wagga Condensed Matter and Materials Meeting in Rotorua (February 4-7). He also gave a series of talks (3 hours in total) at the Virtual Winter School Meeting on (Organizer: Dr. Dirk Andrea, FU Berlin) on *Playing with Polygons – From Graph theory to Fullerenes, Nanotubes and Graphene* (February 17-20).

Seminars and Talks:

- J. Brand gave a lecture on *Strong quantum correlations of a cold atomic gas in experiment and theory* at the Center for Theoretical Physics of Complex Systems, Institute of Basic Sciences Daejeon, South Korea (28 April).
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- M. Piibeleht gave a talk titled "Atoms, relativity and the finite element method: a case study in the Julia language and code reuse" at the Cluster Hui 2020 (Forest and bird lodge – Mount Ruapehu; November 4-6).
- M. Raduban gave a two-hour lecture on *Detecting high energy radiation using solid-state wide band gap materials* at the International School on Photonics and Applications in Hanoi, Vietnam (November 3). The school was held in hybrid-mode where participants who are in Vietnam attended face-to-face while overseas participants joined via Zoom.
- P. Schwerdtfeger gave a lecture on *From the Schrödinger Equation to the Standard Model and Beyond* at Auckland University, Physics Department (November 4).

Poster Presentations:

NA

3. PROFESSIONAL LEADERSHIP AND ADMINISTRATION

Honours and Awards:

- M. Raduban was appointed 0.2 Lectureship at Osaka University. She was also promoted to Senior Lecturer (Range 1) from Lecturer.

Publicity:

- None this year

Appendix 3

1. RESEARCH

Current Areas of Research Activities:

Biomolecular Simulations
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
Force Field Parameterisation
Frequency shifts in atomic clocks
Full Configuration Interaction Quantum Monte Carlo for bosonic systems
Graph theoretical and topological properties of fullerenes
Heterogeneous and Homogeneous Catalysis
High-Pressure Physics
Integrated Nanophotonics
Lattice Sums for extended systems
Macroscopic quantum superpositions
Matter-wave bright solitons
Method of Increments for bulk properties
Multiscale Simulation
Nonlinear waves in Bose-Einstein Condensates
Nonlinear classical and quantum waves in disordered potentials
Nonlinear photonic systems
Non-equilibrium phase transitions
Non-perturbative QED
Nuclear anapole moment
One-dimensional quantum fluids
Optical properties for VUV lasers and scintillators
Parity violation in molecules
Polariton condensate network dynamics
Physics beyond the Standard Model.
Plane-wave pseudopotential development
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
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
Thermodynamics of bulk metals
Theory of functional nanostructures; Spintronics
Topological and Graph Theoretical Aspects of Fullerenes
Transition Metal Catalysis and Theory of Chemical Bonding
Variation of Fundamental Constants in Space-Time

Appendix 4

POST-GRADUATE SUPERVISION

Ongoing PhD Theses:

- Antony Burrows (third year): *On the Calculation of Lennard-Jones-Ingham Coefficients to High Accuracy for Cubic and Hexagonal Lattices*. (Supervisors: P. Schwerdtfeger and S. Cooper).
- Edison Hincapie Florez (third year): *Melting of Molecular Systems* (Supervisors: P. Schwerdtfeger and J. Harrison).
- Morten Piibeleht (third year): *Relativistic and quantum field theoretic studies of many-body atomic and nuclear systems* (Supervisors: P. Schwerdtfeger, P. Bowman).
- Mingrui (Ray) Yang (third year): Full Configuration Interaction Quantum Monte Carlo Calculations on Bosonic Systems (Supervisors: J. Brand and E. Pahl).

Teaching:

- M. Piibeleht demonstrated in the 124.111 (Physics for Life Sciences) labs.
- M. Raduban is course coordinator for the Auckland offering of 124.103 *Biophysical Principles* (semester 1) and gave lectures (12 lectures) and facilitated workshops (6 workshops) in the same course; She also gave lectures (9 lectures) and facilitated workshops (6 workshops) in 124.105 *Physics 1B* (semester 2).
- P. Schwerdtfeger gave lecture courses (20 lectures) on *Environmental Chemistry* within the paper *Environmental and Analytical Chemistry* 123.206 (semester 1), *Introduction to Quantum Theory* (24 lectures) for the *Advanced Physical and Computational Chemistry paper* 123.331 (semester 1).

Other activities:

Papers refereed:

- J J. Brand refereed papers for Physical Review Letters, Physical Review Research, Physical Review A, AVS Quantum Science, New Journal of Physics. M. Raduban refereed in total 13 papers (rejecting 20% of invitations) from 16 different international journals including *Optical Materials*, *Journal of Non-Crystalline Solids*, *Optics Express*, *Optics Communications*, and *Journal of Physics - Materials*.
- P. Schwerdtfeger refereed in total 18 papers (rejecting now 50% of invitations) from 11 different international journals including *Angewandte Chemie*, *Journal of the American Chemical Society* and *Physical Review Letters*.

PhD/MSc and other theses refereed:

- J Brand refereed a PhD thesis from the Department of Physics, University of Auckland.
- M. Raduban examined the confirmation of Sarthak Choudhury (NZIAS), Naina Singhal (School of Food and Advanced Technology), and Dalin Elamana (School of Food and Advanced Technology)

Conference Organisation:

- P. Schwerdtfeger was part of the organizing committee of the REHE (virtual) conference in Assisi (Italy).

Conference Participation:

- See above.

Chairs at Conferences: (none because of Covid-19)

Boards / Editorial Boards / Professional Societies / Memberships:

- J. Brand serves as Vice President of the New Zealand Institute of Physics (NZIP).
- M. Raduban served in the Editorial Board of the journal Applied Sciences and in the Reviewer Board of Micromachines.
- P. Schwerdtfeger served on the Academic Board of Massey University, and occasionally on the MU Research Committee.

Community Outreach:

- M. Raduban demonstrated physics experiments at the Day of Science in Massey University (14 November).

Visits:

- M. Raduban was a visiting Assistant Professor at the Institute of Laser Engineering, Osaka University, Japan from January 16-31 and February 24 – March 31. She was also a visiting researcher at the Institute of Physics, Academy of Sciences of the Czech Republic in Prague, Czech Republic from March 2 – 7.

Exchange Programs:

NA

Grants Refereed:

- P. Schwerdtfeger refereed grants from the Swiss Science Foundation, the German Science Foundation and the Polish Academy of Sciences

Appendix 5

Financial Statement:

Beside financial support from the College of Sciences through SNCS and NZIAS, which covers salaries and administrative support, the following income through internal and external grants was received in 2020 (in NZ\$):

External Grants Received/Continuing:

- J. Brand (PI, Marsden grant)	\$ 102,200
- J. Brand (PI and Theme leader), CoRE grant of the Dodd Walls Centre.	\$ 164,800
- M. Raduban (PI, MURF)	\$ 10,900
- M. Raduban (PI, SREF)	\$ 15,517
- M. Raduban (PI, Osaka University grant; AI Tohoku University grant)	\$ 5,000
- P. Schwerdtfeger and E. Pahl (3rd year Marsden Fund)	\$ 160,000
- P. Schwerdtfeger (2nd year Dumont d'Urville, 12 months)	\$ 40,000

TOTAL **\$ 498,417**

Appendix 5

Staffing

Personnel:

Dist. Prof. Peter Schwerdtfeger (Chemistry and Physics, Director of CTCP, Head of NZIAS)
Prof. Joachim Brand (Physics, Deputy Director of CTCP)
Dr. Marilou Raduban (Lecturer, Physics)

Secretaries:

Vesna Davidovic-Alexander (NZIAS)

External:

Dr. Elke Pahl (Auckland University, Department of Physics)

Honorary Research Fellow:

Prof. Sergej Flach (Korea)

PhD Students:

Antony Burrows (Supervisors: P. Schwerdtfeger, Shaun Cooper and E. Pahl)
Edison Florez (Supervisors: P. Schwerdtfeger and S. Cooper)
Ramin Nikzad (Supervisors: P. Schwerdtfeger, J. Harrison and G. Jameson)
Morten Piibeleht (Supervisors: P. Schwerdtfeger and P. Bowman)
Mingrui (Ray) Yang (Supervisors: J. Brand and E. Pahl)
Sarthak Choudhury (Supervisors: J. Brand and P. Bowmans)

Exchange Students:

None this year because of Covid-19

Postdoctoral/Research Fellows:

Ulrich Ebling (Postdoctoral Fellow)
Paul Jerabek (Humboldt Feodor-Lynen Fellow)
Péter Jeszenszki (Postdoctoral Fellow)
Jan Major (Postdoctoral Fellow)
Jan Mewes (Humboldt Feodor-Lynen Fellow)
Stefanie Mewes (Research Fellow)
Odile Smits (Marsden Postdoctoral Fellow)
Lukas Trombach (Postdoctoral Fellow)

Visitors from other institutions:

Long Term and short term:

Prof. Victor Flambaum (University of New South Wales, Australia)
Dr. Paul Indelicato (Sorbonne Université, Paris, France)
Dr. James Avery (University of Copenhagen, Copenhagen, Denmark)