



# CURRICULUM VITAE

**NAME:****PETER ADOLF SCHWERDTFEGER****QUALIFICATIONS:**

Degree as a chemicotechnical assistant, Chemisches Institut  
Dr. Flad, Stuttgart, Germany, 1973  
Chem. Eng. (grad.), Fachhochschule Aalen, Germany, 1976 (M.Sc.)  
Prediploma Chemistry, Stuttgart, Germany, 1977 (B.Sc.)  
Dipl. Chem., Universität Stuttgart, Germany, 1980 (M.Sc.)  
Prediploma Mathematics, Stuttgart, Germany, 1983 (B.Sc.)  
Dr. rer. nat., Universität Stuttgart, Germany, 1986 (Ph.D.)  
Habilitation and venia legendi, Philipps-Universität Marburg, Germany, 1995

**PROFESSIONAL  
AFFILIATIONS:**

President of the New Zealand Humboldt Association  
Fellow of the Royal Society New Zealand  
Fellow of the New Zealand Institute of Chemistry  
Elected Council Member of The Royal Society New Zealand  
Member of the American Chemical Society, the Gesellschaft  
Deutscher Chemiker, the Deutscher Hochschulverband, the  
American Physical Society, and the Arbeitsgemeinschaft  
Theoretische Chemie  
Board: Asian-Pacific Association of Theoretical and Computational Chemist

**PRESENT POSITION:**

Professor of Theoretical Chemistry (since March 2004), Massey University  
Privatdozent, Philipps-Universität Marburg (since Dec 1995)  
Deputy Director of the Institute of Fundamental Sciences (since Dec 2004)  
Director of the Centre of Theoretical Chemistry and Physics (since 2006)

**PREVIOUS POSITIONS:**

Teacher in chemistry and physics for intermediate schools,  
Stuttgart, Germany, 1980-81  
Taxi-Driver, Stuttgart, Germany, 1981-1987  
Teacher in atomic physics and theory of relativity at  
public high schools, Stuttgart, Germany, 1982-87  
Computer software analyst, Institut für Theoretische Chemie,  
Universität Stuttgart, Germany, 1981-87  
Postdoctoral Fellow, Department of Chemistry,  
University of Auckland, 1987-89  
Research Fellow, School of Engineering, The University  
of Auckland, 1989  
Research Fellow, School of Chemistry, The Australian  
National University, Canberra, Australia, 1989-1991  
Lecturer, Department of Chemistry, University of  
Auckland, New Zealand, 1991-1992  
Senior Lecturer, Department of Chemistry, University of  
Auckland, New Zealand, 1993-1995  
Visiting Professor in Marburg, 1994,95  
Associate Professor, Department of Chemistry, University of  
Auckland, New Zealand, 1995-1998  
Professor (personal chair) Department of Chemistry, University of  
Auckland, New Zealand 1999-2003

**AWARDS/PRIZES:**

Alexander von Humboldt Feodor Lynen Award  
(Alexander von Humboldt Stiftung, Bonn) 1987  
Prince & Princess of Wales Science Award  
(Royal Society of New Zealand) 1988 (NZ\$ 2,500)  
SGS Prize for excellence in basic research (NZ\$ 1,000)  
(New Zealand Institute of Chemistry) 1994  
Marsden Fund Award 1996 (NZ\$ 570,000 for research)  
Fellow of the Royal Society New Zealand, 1997  
Fellow of the New Zealand Institute of Chemistry, 1998  
Marsden Fund Award 1999 (NZ\$ 590,000 for research)  
Hector Medal for undertaken work of great scientific or technological  
merit and outstanding contribution to the advancement of the  
particular branch of science (Royal Society New Zealand) 2001  
James Cook Fellowship 2001 (2 years)  
Marsden Fund Award 2003 (NZ\$ 630,000 for research)  
Marsden Fund Award 2006 (NZ\$ 690,000 for research)

**BUSINESS ADDRESS:**

Institute of Fundamental Sciences, Massey University  
(Albany Campus), Private Bag 102904, North Shore MSC,  
Auckland. Telephone: (64-9) 443 9780,  
FAX: (64-9) 443 9779  
email: p.a.schwerdtfeger@massey.ac.nz

**PERSONAL DETAILS:**

**Nationality:** German, NZ citizen

**KEYNOTE/PLENARY (K) and INVITED (I) CONFERENCE LECTURES :**

1. Adriatico conference on "Relativistic Many-Body Problems", Trieste (Italy), June 30 - July 4, 1986. (I)
2. Winter School in Theoretical Chemistry on "DNA, Heavy Metals and their Interactions",  
Helsinki (Finland), December 17 - December 20, 1990. (K)
3. European Research Conference on "Relativistic Effects in Heavy-Element Chemistry and Physics",  
DeHaan (Belgium), June 10 - June 14, 1993. (K)
4. 8th International Congress of Quantum Chemistry, Prague, Czech Republic, June 19 - 23, 1994. (K)
5. Pseudopotential Workshop, Toulouse, France, May 1994. (K)
6. Conference on Computational Chemistry, Mariapfarr (Austria), March, 1995. (K)
7. Pacific/Chem Conference, Hawaii (U.S.A.), December 1995 (K)
8. International Conference on the Chemistry of Gold, Hanau (Germany), June 16-20, 1996. (K)
9. 4th World Congress of Theoretically Orientated Chemists, WATOC, Jerusalem (Israel), July 7-12, 1996. (K)
10. 5th Conference of Current Trends in Computational Chemistry, Jackson (USA), November 1-2, 1996. (K)
11. Research Conference on Relativistic Effects on Structure, Dynamics and Spectroscopy,  
March 8 - 13, 1997, Granada (Spain). (K)
12. Academy of Sciences Annual Speaker, Budapest, December 1997.
13. Deutsche Forschungsgemeinschaft, "Schwerpunktsprogramm Relativistische Effekte", Kassel,  
May 10-12, 1998. (K)
14. 12th European Symposium on Fluorine Chemistry, Berlin, August 29-September 2, 1998. (K)
15. European Congress on Electron Gas Phas Diffraction, Blaubeuren, June 19-23, 1999. (K)

16. 8<sup>th</sup> International Conference on the Applications of Density Functional Theory to Chemistry and Physics, Rome, September 6-10, 1999. (I)
17. 35<sup>th</sup> Symposium for Theoretical Chemistry, September 12-16, Freiberg (Germany), 1999. (K)
18. American Chemical Society Southeast Regional Meeting, SERMACS-99, Knoxville (USA), October 17-20, 1999. (K)
19. 11th RACI Conference, ANU Canberra, 6-11 February 2000. (K)
20. Xth International Congress on Quantum Chemistry, Menton (France), June 5-10, 2000. (K)
21. Symposium on Heavy Metal Chemistry and Physics, Presqu'île de Giens (France), May 30 – June 3, 2000. (K)
22. Symmetry 2000, Wenner-Gren Foundations International Symposium, September 13-16, 2000 (K)
23. Pacificchem 2000 meeting, December 14 – 19, 2000, Honolulu (Hawaii) (K and I)
24. International School of Crystallography, 32<sup>nd</sup> Course: Strength from Weakness. Structural Consequences of Weak Interactions in Molecules, Supermolecules, and Crystals. Erice (Sicily), 23 May – 3 June, 2001. (K)
25. Finish Symposium on Quantum Chemistry, Kuusamo (Finland), 11 – 17 June, 2001. (K)
26. European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Workshop on Very Heavy Nuclear Systems, Trento (Italy), 9 – 14 July (2001). (K)
27. ASR2001 Conference: Advances in Heavy Element Research, Tokai, Ibaraki (Japan), November 13-15 (2001). (K)
28. AvH meeting: Scholarship and Research in Turbulent Times, Sydney (Australia), December 7-9 (2001). (K)
29. AGICHEM2002, Inorganic Chemistry, Munich (Germany), April 7-10 (2002). (K)
30. Symposium on Relativistic Effects in Heavy-Element Chemistry, Berlin (Germany), 28. – 30. 7 (2003) (K)
31. Gold2003 Conference, Vancouver (Canada), 28.9. – 1.10 (2003) (K)
32. TAN03 – Conference on Superheavy Elements, Napa Valley (USA), 16.-20.10 (2003) (K)
33. RACI Conference on Physical Chemistry, February 1-5, 2004, Hobart (Tasmania). (K)
34. 1<sup>st</sup> Asian Pacific Conference on Theoretical and Computational Chemistry, May 12-15, 2004, Okazaki (Japan). (K)
35. Symposium for Theoretical Chemistry, September 19-23, 2004, Suhl (Germany). (K)
36. 2004 NZIC Inorganic and Organometallic Specialist Group Conference, Portage, December 5-8, 2004 (New Zealand). (K)
37. Second Asian Pacific Conference on Theoretical & Computational Chemistry, May 2-6, 2005, Bangkok (Thailand). (K)
38. 19<sup>th</sup> Colloquium on High Resolution Molecular Spectroscopy, September 11-16, 2005, Salamanca (Spain). (K)
39. ICCMSE 2005. International Conference of Computational Methods in Sciences and Engineering, 21-26 October, Loutraki (Greece). (K, 2 lectures)
40. Otago Lasers and Applications Research Theme (LART), November 14, 2005, Dunedin. (K)
41. Pacificchem 2005 meeting, December 14 – 19, 2005, Honolulu (Hawaii) (K, 2 lectures)
42. Theoretical Chemistry Symposium, Rauischholzhausen (Marburg), April 11-13, 2006 (K)
43. ACS National Meeting, San Francisco (USA), September 10-14, 2006 (K)
44. Relativistic Effects in Heavy Elements (REHE) 2007 Conference, Ottrott, France, March 21-25, 2007 (K)
45. Molecular Quantum Mechanics - Analytic Gradients and Beyond, An International Conference in Honor of Professor Peter Pulay, May 29 - June 3, 2007 (Chair)
46. Invited to two more international conferences in 2007

#### COMPUTER EXPERIENCE:

Experience in large scale computing and in soft- and hardware developments on CYBER, IBM, VAX, CRAY and FUJITSU computers, experience in FORTRAN, PASCAL, C and C++, several assembler languages, HTML, SHELL-programming, several operating systems including the AIX RISC6000 and UNICOS Cray operating systems.

#### RESEARCH, BSc, MSc AND PhD STUDENTS AND POSTDOCTORAL FELLOWS

##### BSc, MSc and PhD Students:

- 1) Dr. Patricia Hunt, PhD student 1993-1997.  
Title: *Jahn-Teller Distortions in Molecules Containing Group 15 Elements.*
- 2) Dr. Michael Seth, MSc student 1993, PhD student 1994-1997.  
MSc Title: *The Effects of Vibration and Rotation on the Molecular Properties of Diatomic Molecules.*  
PhD Title: *The Chemistry of the Superheavy Elements.*
- 3) Mrs. Fiona Esther Cooke, BSc (hon.) student 1995  
BSc title: *A Theoretical Study of the Reaction  $MF_4^- \rightarrow MF_2^- + F_2$  for Group 11 Elements.*

- 4) Dr. Reuben Brown, BSc (hon.) student 1996, PhD student 1997-2001.  
BSc title: *Semi-empirical Calculations on Nitro-Heteroaromatic Quaternary Amines.*  
PhD title: *Theoretical Studies of Gold Compounds.*
- 5) Mr. Ivan Lim, MSc student, 1997-98, PhD student 1999-2005.  
MSc title: *Electric Polarizabilities of Group 1 Elements from H to Element 119.*  
PhD title: *Small-core pseudopotentials for Group 1 and 2 elements.*
- 6) Mrs. Silke Pelzer, MSc student 1999  
MSc title: *Jahn-Teller distortions in organic ring systems.*
- 7) Mrs. Nicola Gaston, BSc (hon.) student 2001, PhD student 2002-2005  
BSc title: *QED effects in K- and L-shell ionisation potentials of superheavy elements*  
PhD title: *Large cluster systems – Towards nanosized materials*
- 8) Mr. Behnam Assodollahzadeh, PhD student 2004  
PhD title: *Gold Nanostructures*
- 9) Mr. Brian Vest, PhD student 2005  
PhD title: *Cluster of CrCl<sub>2</sub>*
- 10) Mr. Christian Thierfelder, PhD student 2005  
PhD title: *Parity Violation in Chiral Molecules*
- 11) Mr. Andreas Hermann, PhD student 2005  
PhD title: *Solid state calculations of H<sub>2</sub>O*
- 12) Mr. Susan Biering, PhD student 2005  
PhD title: *The Solid State of Group 12 Oxides and Relativistic Effects*

**Fellows:**

- 1) Dr. Malkhaz Meladze, Research Fellow 1997/98.  
Title: *Theoretical Models for the Treatment of He Inside Buckminsterfullerene.*
- 2) Mr. Joerg Rissler (PhD student from Prof. Baessler's Group in Marburg), financed by the Graduiertenkolleg of the Phillips University Marburg; Germany, 1998.  
Title: *UV Spectra of Organic Polymers.*
- 3) Mr. Joern Thyssen (PhD student from Prof. Jensen's Group in Denmark), financed by Odense University; 1999.  
Title: *Fully relativistic treatment of electric field gradients and higher derivatives.*

**Exchange Students:**

- 1) Mr. Thomas Szyperski (Exchange Student from the TU Munich), Fellow of the Studienstiftung des Deutschen Volkes, Germany; 1988/1989.  
Title: *Organometallic Trioxo Group 7 Compounds.*
- 2) Mrs. Karin Wichman (Exchange Student from the Philipps Universität Marburg), Marburg, Germany; 1998.  
Title: *The Inversion Potential of NH<sub>3</sub>.*
- 3) Mr. Matthias Lein (Exchange Student from the Philipps Universität Marburg), Marburg, Germany; 1999-2000.  
Title: *Porphyrine Systems.*
- 4) Mr. Andreas Kühn (Exchange Student from the Humboldt Universität Berlin), Berlin, Germany; 2000.  
Title: *Electroweak Interactions.*
- 5) Mr. Johannes Gierlich (Exchange Student from the Philipps Universität Marburg), Marburg, Germany; 2001.  
Title: *Electroweak Interactions.*
- 6) Mr. Ralf Tonner (Exchange Student from the Philipps Universität Marburg), Marburg, Germany; 2001.  
Title: *Group 18 Cluster.*
- 7) Mr. Radovan Bast (Exchange Student from the Philipps Universität Marburg), Marburg, Germany; 2002.  
Title: *Field Gradients from DFT.*
- 8) Mr. Christoph Jacob (Exchange Student from the University of Karlsruhe), financed by the Studienstiftung des Deutschen Volkes; 2003.  
Title: *Simulation of Gold Cluster.*
- 9) Mr. Philipp Moerschel (Exchange Student from the Philipps Universität Marburg), financed by the Philipps Universität Marburg, 2004  
Title: *Simulation of Cesium Cluster.*
- 10) Mr. Christian Olendrowitz (Exchange Student from the Humboldt University Berlin)  
Title: *Peptide Simulations*

- 11) Mr. Daniel Benker (Exchange Student from the LMU Munich, Germany)  
Title: Polarizabilities of Sn Cluster
- 12) Mr. Sascha Schäfer (Exchange Student from the TU Darmstadt, Germany)  
Title: Polarizabilities of Sn Cluster

**Postdoctoral Fellows:**

- 1) Dr. Josef Ischtwan (from L.Radom's group, Canberra), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 1991-1993.  
Title: *Permutation Invariant Hypersurfaces.*
- 2) Dr. Thomas Fischer (from J.Aimlőf's group, Minnesota), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 1994-1996, Research Fellow since 1997.  
Title: *Electronic Structure of Tetrapyrrole Compounds, Vibrational Anharmonicity Effects in Polyatomic Molecules.*
- 3) Dr. Hinne Hetteema (from Nieuwpoort's group, Groningen), AURC Postdoctoral Fellow; 1995-1996.  
Title: *Electric Properties of Cluster Compounds.*
- 4) Dr. Klaus Hübler (from Becker's group, Stuttgart), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 1995-1996.  
(together with Warren Roper and James Wright)  
Title: *Organometallic Compounds of Osmium.*
- 5) Dr. Markus Pernpointner (from Preuss' group, Stuttgart), Marsden Postdoctoral Fellow for 1997/98  
Title: *Theoretical Treatment of Field Gradients and Nuclear Quadrupole Moments.*
- 6) Dr. Ralf Wesendrup (from H.Schwarz group, Berlin), DFG Postdoctoral Fellow for 1997/98  
Title: *Heterogeneous Catalysis on Pt-Surfaces.*
- 7) Dr. Jon Laerdahl (from K.Faegri's group, Oslo) Marsden Postdoctoral Fellow 1998/99.  
Title: *Electrostatic Interactions (Z-boson Exchange) and Biomolecular Homochirality.*
- 8) Dr. Michael Möhlen (from K.Dehnicke's group, Marburg), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 1999-2000.  
(together with Warren Roper and James Wright)  
Title: *Organometallic Compounds of Osmium.*
- 9) Dr. Tilo Söhnel (Dresden), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 2000-2001.  
Title: *Solid state computational chemistry*
- 10) Dr. Holger Hermann (Prof. Boche's group, Marburg), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 2000-2002.  
Title: *Metal-Metal Interactions*
- 11) Dr. Gloria E. Moyano (Bogota, Columbia), Marsden Fellow (2001-2002)  
Title: *Many body potentials for metal clusters, cluster dynamics and phase transitions*
- 12) Dr. Tobias Bollwein (Bogota, Columbia), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 2001-2002.  
(together with P. Brothers).  
Title: *Porphyrine Systems*
- 13) Dr. Tony Hammerl (Prof. Klapötke's group, LMU Munich, Germany), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 2002-2003  
Title: *Nitrogen Rich Explosives*
- 14) Dr. Robert Krawczyk (TU Munich, Germany), Postdoctoral FEODOR-LYNEN Fellow of the Alexander von Humboldt Foundation, Bonn, Germany; 2003-2005  
Title: *Gold Nano-Structures*
- 15) Dr. Gloria E. Moyano (Bogota, Columbia), Marsden Fellow (2006)  
Title: *Rare Gas Clusters*
- 16) Dr. Matthias Lein (Prof. Frenking's group, Marburg, Germany), Postdoctoral Marsden Fellow 2004-2006  
Title: *Homogeneous Catalysis of Au(III)*
- 17) Dr. Elke Pahl (Prof. Fulde's group, MPI Dresden, Germany), Postdoctoral Fellow 2006-2009  
Title: *Simulation of Mercury Melting*
- 18) Dr. Detlef Figgen (Prof. Stoll's group, Stuttgart, Germany), Postdoctoral Marsden Fellow 2007-2009  
Title: *Parity Violation in Molecules*

**Long Term Visitors to our research group (since 1991):**

Prof. Roald Hoffman (Cornell), Prof. Pekka Pyykkö (Helsinki), Prof. N.Rösch (Munich), Dr. Lars Bengtsson-Kloo (Lund), Dr. Karl-Wilhelm Klinkhammer (Stuttgart), Prof. Dieter Schuch (Frankfurt), Prof. Helmut Schwarz (Berlin), Prof. Jan Evert Baerends (Amsterdam), Prof. Bob Compton (Tennessee), Profs. Istvan and Magdi Hargittai (Budapest), Prof. Mike Mingos (Imperial College), Prof. Ulrich Müller-Herold (ETH Zürich), Prof. Tom W. Klapötke (LMU Munich), Prof. R. Steudel (TU Berlin), Dr. Joern N. Greif (Marburg), Prof. W. Thiel (MPI Mülheim), Prof. Trond Saue (Mülheim), Prof. Uzi Landman (Georgia, USA), Prof. Burkhard Fricke (Kassel), Dr. Josef Anton (Kassel), Prof. Ditmar Kolb (Kassel), Prof. Ian Hamilton (Canada).

**RESEARCH GRANTS (since 1991):**

1. Auckland University Research Committee (AURC) 1991-2003 (total of 33 grants)	NZ\$	644,848
2. Lottery Science 1991	NZ\$	20,000
3. Major Equipment Grant, University of Auckland 1993	NZ\$	33,000
4. Auckland University Postdoctoral Fellowship 1994/95	NZ\$	74,000
5. Lottery Science, AURC and VC (high-performance super computer, together with P. Hunter and J. S. McFeaters) 1996	NZ\$	1,000,000
6. Marsden Fund (1996-98)	NZ\$	570,000
7. Geo2 Company (Australia) 1998-00	NZ\$	47,600
8. Marsden Fund (2000-03)	NZ\$	590,000
9. New Economy Research Fund (2000-2001) (together with W. R. Wilson and W. A. Denny)	NZ\$	23,800
	NZ\$	1,050,000
10. Research Infrastructure Fund	NZ\$	45,000
11. CAPEX Fund, Auckland (2001, together with P. Hunter)	NZ\$	300,000
12. CAPEX Fund, Auckland (2002)	NZ\$	150,000
12. Distinguished research visitor award (2001)	NZ\$	6,750
13. International research collaboration award (2001)	NZ\$	4,000
14. James Cook Award (2001-2003)	NZ\$	190,000
15. VC Development Fund (2002)	NZ\$	50,000
16. Marsden Fund (2003-06)	NZ\$	630,000
17. Massey University Establishment grant (2004)	NZ\$	190,000
18. Royal Society DFG Programme	NZ\$	24,000
19. College of Sciences Minor Equipment Fund	NZ\$	14,000
20. ISAT Travel grant 2006/2007	NZ\$	5,400
21. Marsden Grant 2007-2009	NZ\$	870,000
22. Dumont D'Urville 2007	NZ\$	3,900
	<b>TOTAL</b>	<b>NZ\$ 6,540,278</b>

Numerous travel grants not listed here from the European Science Foundation, Deutsche Forschungsgemeinschaft, Alexander von Humboldt Foundation and the NZ/FRG Agreement.

**CONFERENCE ORGANIZATION:**

- 1) *Australian and New Zealand Institute of Chemistry Conference*, Auckland, December 1992.
- 2) *Oils and Fats*, Auckland, November 1997
- 3) *Organometallic Chemistry in the South Pacific*, Auckland, January 1999.
- 4) *Pacificchem*, Hawaii, December 2000
- 5) 1<sup>st</sup> Joint Australian – New Zealand Humboldt Colloquium, 2004.
- 6) *Pacificchem*, Hawaii, December 2005
- 7) NZ/FRG Workshop on Superheavy Elements, Auckland, May 28/29, 2005.
- 8) Chair for the *New Zealand Institute of Chemistry Conference*, Rotorua, December 2006.
- 9) Chair for the Relativistic Symposium, ICCMSE, Crete, October 2006.
- 10) Chair for the ACS Boston Meeting, Nuclear Chemistry Subdivision, Boston, August 2007.

**EDITORIAL BOARDS, REVIEWER (MAJOR JOURNALS, RESEARCH GRANTS):**

Editorial Board for Journal of Computational Chemistry, Journal of Computational Methods in Sciences and Engineering, and Structural Chemistry

Advisory Board for Asian/Pacific Theoretical and Computational Chemistry Association.

Reviewer for many journals including Nature, Journal of the American Chemical Society, Angewandte Chemie, Chemistry - A European Journal, Organometallics, Physical Review A, Physical Review Letters, Journal of Chemical Physics, Journal of Physical Chemistry, Inorganic Chemistry, Journal of Organic Chemistry, Theoretica Chimica Acta, Account of Theoretical Chemistry, Chemical Physics, Phys. Chem. Chem. Phys., Chem. Phys. Chem., International Journal of Quantum Chemistry, J. Mol. Struct., Struct. Chem., Faraday Transactions, Computational Chemistry, Journal of Materials Chemistry, Australian Journal of Chemistry, Physics Letter A, National Science Foundation (U.S.A.), ANU Supercomputer Facility, FoRST New Zealand, Australian Research Council, Marsden Fund.