

Professor Peter R. Taylor

Curriculum vitae

Vice-Dean for Information Technology and Professor of Chemistry
Health Science Platform
Tianjin University, Tianjin, China
h-index: 67 (Google Scholar)

Date of birth: 14 February 1952
Place of birth: Bromley, Kent, England
Citizenship: British



Family status: widowed (Valerie Taylor), two sons; recent partner Dr Natalie Gilka (deceased)

Contact information:

A: Health Science Platform M: +86 13312170897
A203, Bldg 24 +44 (0)7561 300740
Tianjin University E: pete@tju.edu.cn
92 Weijin Rd, Nankai Dist. S: qc_wizard
Tianjin 300072, CHINA

Academic qualifications:

1974 B. Sc. (Hons. I), Sydney University
Department of Theoretical Chemistry

1978 Ph. D., Sydney University
Department of Theoretical Chemistry

Positions held:

2015–2017 Visiting Professor,
Department of Chemistry,
Aarhus University, Denmark

2015–2017 Honorary Professor,
School of Chemistry,
University of Melbourne, Australia

2010–2015 Director,
Victorian Life Sciences Computation Initiative,
University of Melbourne, Australia
and
Adjunct Professor,
School of Chemistry,
University of Melbourne, Australia

2002–2010 Royal Society Wolfson Professor of Chemistry
and Chief Scientist, Centre for Scientific Computing,
University of Warwick, UK

1999–2002 Professor,
Department of Chemistry, University of California, San Diego

1997–2002 Deputy Director,
San Diego Supercomputer Center

1994–1997 Associate Director for Science,
San Diego Supercomputer Center

1994–1999 Adjunct Professor,
Department of Chemistry and Biochemistry,
University of California, San Diego

1992–1994 Senior Staff Scientist,
San Diego Supercomputer Center

1985–1992 Research Scientist,
ELORET Institute, Palo Alto, California USA
Supported by NASA Ames Research Grant NCC 2-371

1981–1985 Research Scientist,
CSIRO Division of Chemical Physics, Melbourne, Australia
(Promoted to Senior Research Scientist July 1983)

1984–1985 Honorary Research Associate,
Department of Chemistry, Monash University, Melbourne, Australia
(Honorary position held simultaneously with the CSIRO appointment)

1979–1980 Post-doctoral research fellow,
Lehrstuhl für Theoretische Chemie der Universität Karlsruhe, West Germany 1979 – 1980
Alexander von Humboldt-Stiftung Research Fellowship

1978–1979 Post-doctoral research fellow,
Chemical Center, Lund, Sweden
Feb. 1978 – Jan. 1979 CSIRO Post-doctoral Research Fellowship
Feb. 1979 – Aug. 1979 Supported by a grant from the Swedish Natural Science Research
Council (NFR)

1975 Graduate study visitor at CSIRO Division of Chemical Physics, Melbourne, Australia

Research:

My main interest in research throughout my career has been the electronic structure of molecules: quantum chemistry, both purely theoretical and computational. Partly as a result of the latter, I have been extensively involved in high-performance computing, both as a researcher and also in

management and strategic development. I have published over 190 papers in the peer-reviewed literature, with an *h*-index of 67.

Supervision:

I have supervised or co-supervised twelve postdoctoral fellows, sixteen PhD students, and eight project students. I should note that the positions I held at CSIRO and NASA Ames offered no opportunities to supervise PhD or project students, and during my time at UCSD and at VLSCI I refused to take PhD or project students, because of my management responsibilities.

Teaching:

I have taught at all undergraduate levels (freshman – senior, or 1st – 4th year), including physical chemistry (structure and bonding, spectroscopy of atoms and molecules), structural inorganic chemistry, and theoretical and computational chemistry (lectures and hands-on classes). At the graduate level I have taught advanced quantum chemistry, applications of group theory in molecular quantum mechanics, and a master's level course on computational linear algebra.

I have also taught at the European Summer School in Quantum Chemistry since its inception (in 1989) and have organized a master's level training centre in high-end computing with funding from the UK research Council (EPSRC).

Professional Societies:

American Chemical Society
American Physical Society
Association for Computing Machinery
Society for Industrial and Applied Mathematics
American Association for the Advancement of Science

Honours, Special recognition:

Conference in honour of 60th birthday, Zürich, 2012
Wolfson Research Merit Award, Royal Society of London, 2002–2007
Robert S. Mulliken Lecture, University of Georgia, 1998
Finalist, Computerworld-Smithsonian Award for Breakthrough Computational Science, 1993
Co-recipient, NASA Group Achievement Award, 1988
Guest research scientist, Minnesota Supercomputer Institute, 1986–1992
Associate, NASA Ames Research Center, 1984–1985
Alexander von Humboldt Fellow, 1979–1980

Journal Boards:

Editorial Board, *Molecular Physics* 2015–2017
Editorial Board, *Journal of Computational Methods in Sciences and Engineering* 2000–2002
Editorial Board, *Progress in Theoretical Chemistry and Physics* 1999–2005
Principal Editor, *Computer Physics Communications* 1998–2005
Advisory Editorial Board, *The Journal of Chemical Physics* 1994–1996

Recent Publications

- [182] K. E. Yousaf and P. R. Taylor, On the electronic structure of small cyclic carbon clusters, *Chem. Phys.* **349**, 58 (2008).
- [183] P. Dahle, T. Helgaker, D. Jonsson, and P. R. Taylor, Second-order Møller-Plesset calculations on the water molecule using Gaussian-type orbital and Gaussian-type geminal theory, *PCCP* **10**, 3377 (2008).
- [184] N. Gilka, P. R. Taylor, and C. M. Marian, Electron spin-spin coupling from multireference configuration interaction wave functions, *J. Chem. Phys.* **129**, 044102 (2008).
- [185] B. O. Roos, V. Veryazov, J. Conradie, P. R. Taylor, and A. Ghosh, Not innocent: the verdict from ab initio multiconfigurational second-order perturbation theory on the electronic structure of chloroiron corrole, *J. Phys. Chem. B* **112**, 14099 (2008).
- [186] V.-A. Glezakou and P. R. Taylor, On the electron affinity of B₂, *Eur. J. Mass. Spectrom.* **15**, 337 (2009).
- [187] P. R. Taylor, Configurations of equivalent electrons, *J. Phys. Chem. A* **113**, 12632 (2009).
- [188] D. Ganyushin, N. Gilka, P. R. Taylor, C. M. Marian, and F. Neese, The Resolution of the Identity Approximation for Calculations of Spin-Spin Contribution to Zero-Field Splitting Parameters, *J. Chem. Phys.* **132**, 144111 (2010).
- [189] G. M. Arantes and P. R. Taylor, Approximate multiconfigurational treatment of spin-coupled metal complexes, *J. Comput. Theor. Chem.* **6**, 1981 (2010).
- [190] R. Rios-Font, M. Sodupe, L. Rodriguez-Santiago, and P. R. Taylor, The role of exact exchange in the description of Cu²⁺-(H₂O)_n (n=1-6) complexes by means of DFT methods, *J. Phys. Chem. A* **114**, 10857 (2010).
- [191] N. Gilka, J. P. Solovej, and P. R. Taylor, On the behaviour of the Hartree-Fock energy at short internuclear distances, *Int. J. Quantum Chem.* **111**, 3324 (2011).
- [192] X. Huang, P. R. Taylor, and T. J. Lee, Highly accurate quartic force fields, vibrational frequencies, and spectroscopic constants for cyclic and linear C₃H₃⁺, *J. Phys. Chem. A* **115**, 5005 (2011).
- [193] K. Aidas et al., DALTON quantum chemistry program system, *WIREs: Comp. Mol. Sci.* **4**, 269 (2014).
- [194] P. R. Taylor, Lossless compression of wave function information: a gzip for quantum chemistry, *J. Chem. Phys.* **139**, 074113 (2013).
- [195] K. J. Catani, J. A. Sanelli, V. Dryza, N. Gilka, P. R. Taylor, and E. J. Bieske, Electronic spectra of the propargyl cation tagged with Ne and N₂, *J. Chem. Phys.* **143**, 184306 (2015).
- [196] P. R. Taylor, Reflections on the MOLECULE integral program (and its developer), *Mol. Phys.* **115**, 2043 (2017).