CURRICULUM VITAE

Dr. Michael David Towler

Senior Research Associate/ Royal Society Research Fellow (University of Cambridge)
College Lecturer (Emmanuel College, Cambridge)
Senior Research Associate (University College London)
Director (Apuan Alps Centre for Physics, Italy)

Mike Towler is a theoretical physicist who for almost 20 years has worked in the Theory of Condensed Matter group at Cambridge University's Cavendish Laboratory, and in recent years also part time at University College, London. His research is largely concerned with the development of highly accurate quantum-mechanical methods useful in understanding and predicting the properties of matter. He is a specialist in massively parallel computing, and routinely develops and runs calculations on some of the most powerful machines in the world. He is an author of over sixty scientific articles and book chapters, and has written a number of widely used international-class software programs, including the leading quantum Monte Carlo code 'CASINO'. For many years the simultaneous holder of a prestigious Royal Society Research Fellowship in the Cavendish and a permanent College Lectureship at Emmanuel College, Cambridge, he is also the founder and director of the internationally known 'Apuan Alps Centre for Physics' in Italy, where he has hosted over twenty major events including his own series of computational chemistry summer schools. An experienced public speaker and educator, he has given numerous invited talks all over the world along with various lecture courses and thousands of small-group supervisions over many years in Cambridge.

Main work addresses: Keil Art Bronze Gallery, via dei Fossi 3/5r, Florence, Italy, *and* Apuan Alps Centre for Physics, via del Collegio 22, Vallico di Sotto, 55021 Fabbriche di Vallico, Italy *and* TCM Group, Cavendish Laboratory, Cambridge University, 19 J.J. Thomson Avenue, Cambridge CB3 0HE, U.K. (where I currently have 'Visitor' status).

Home address: *removed for publication*

Telephone: *removed for publication*

Email: mdt26 'at' cam.ac.uk

Relevant web pages:
`vallico.net/casinoqmc/` (Quantum Monte Carlo)
`vallico.net/tti/tti.html` (Apuan Alps Centre for Physics)

Secondary and university education

Bolton School
4 'A' levels – all grade A (1988) [one awarded national prize for best 'A' level paper in U.K.]
1 'S' level – grade 1 (1988)

University of Bristol
B.Sc. 1st class (1991)
Ph.D. in computational physics (1994)

Academic positions

University of Torino
Dipartimento di Chimica Teorica
- EU HCM Individual Research Fellowship (Nov 1994–Dec 1996)

University of Cambridge
Theory of Condensed Matter Group, Cavendish Laboratory
- Postdoctoral Research Associate (Dec 1996–Oct 2000)
- Lloyd's Fellow (Oct 2000–Oct 2002)
- Royal Society Research Fellow (Oct 2002–Sep 2010)
- EPSRC Senior Research Associate (Oct 2013–Oct 2015)

University of Cambridge
Emmanuel College
- College Lecturer (Oct 2002–April 2012). Post permanent but voluntarily given up.

University College London
- EPSRC Senior Research Associate (Oct 2010–Oct 2015)

Additional academic and business experience

BASF
Ludwigshafen, Germany, summer placement (2 months, 1992)

Pacific Northwest Laboratory
Washington, U.S.A., Laboratory Fellowship (2 months, 1994)

Daresbury Laboratory
Computational Materials Science Group, multiple summer placements (1991–94)

Schools and training workshops
- "*European summer school in quantum chemistry*" (Tjörnarp, Sweden, 1995)
- "*Local density functional and beyond*" (Condensed matter physics research workshop, Trieste, Italy, 1996)
- "*Quantum chemistry and molecular properties*" (Fourth Sostrup summer school, Denmark, 1996)
- "*Physics of insulators* (Aspen Centre for Physics, Aspen, U.S.A., 3 weeks, 1998)
- "*Best practice in HPC software development*" (Oxford, 2009)
- "*Innovation and the business of science*" (Three modules: Science and the Economy, Leadership, Entrepeneurship at the Royal Society, London, 2009)
- "*Introduction to CUDA programming on NVIDIA GPUs*" (Numerical Algorithms Group, Oxford, 2011)

Conference and summer school organization

Organized international workshops entitled "*Diffusion Monte Carlo*" in 2002 at CECAM, Lyon, France, and "*The quantum Monte Carlo method*" at RMIT University, Melbourne, Australia in 2003.

Created and developed own science institute, conference centre, and events venue - the 'Apuan Alps Centre for Physics' - in the mountain village of Vallico Sotto, Italy. Since it opened in 2004 more than 450 scientists from around the world have passed through the Institute (many of them repeatedly) whilst attending the twenty-two major events organized there.

Originator and organizer of the conference series "*Quantum Monte Carlo in the Apuan Alps*" held each year since July 2005 in Vallico Sotto, and of the annual "*Quantum Monte Carlo*

and the CASINO program" summer schools at the same venue beginning in August 2006. Institute also hosted several independent workshops "*KKR and many-body applications*" and "*Nucleic Acids Function*", along with the 2006 "*CASTEP Festival*". In late August 2010 organized a workshop "*21st-century directions in de Broglie-Bohm theory and beyond*" with Antony Valentini, when around sixty people visited Vallico Sotto including many leading physicists.

MEDIA

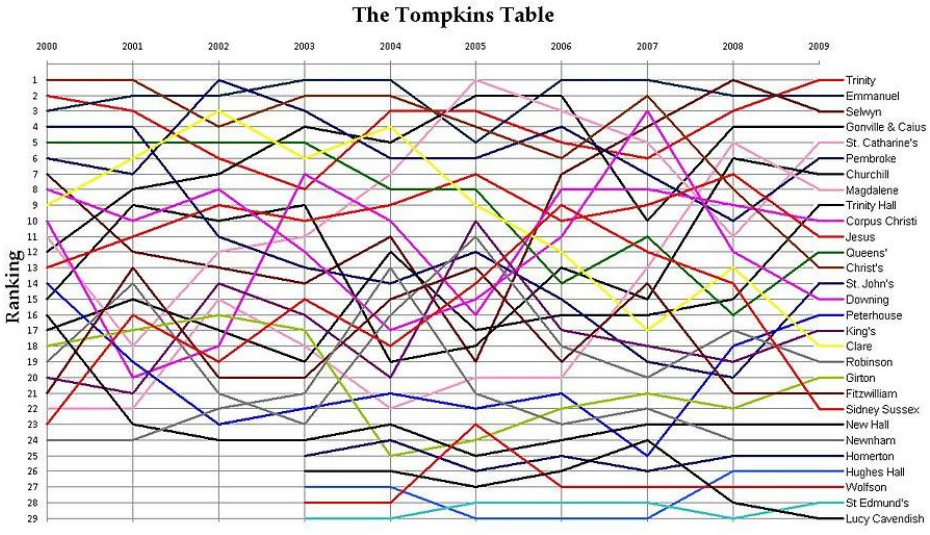
Was invited by the BBC in October 2010 to be a contributing presenter for their new series "*The Wonders of the Universe*".

TEACHING AND SUPERVISING EXPERIENCE

1997-2012 : Undergraduate tutorials in Cambridge in the following subjects: Mathematics for Natural Sciences (1st and 2nd years); IA and IB physics, including Thermodynamics, Oscillations, Waves and Optics, Electromagnetism, Statistical Physics, Quantum Physics (1st and 2nd year); Quantum Mechanics, Solid State Physics, Theoretical Physics (3rd and 4th years). For ten years I held a permanent position as College Lecturer at Emmanuel College - one of only two staff responsible for the teaching of physics.

As is well known, Cambridge is consistently ranked in the top few universities in the world and, according to the Tompkins Table (`en.wikipedia.org/wiki/Tompkins_Table`) which ranks the academic results of the twenty-nine Cambridge Colleges, Emmanuel is ranked first equal with Trinity on average over the years since 1997, with Emmanuel being particularly strong in science and Trinity in the arts and humanities. The years I was active in the college are highlighted in yellow in the table of rankings below.

College	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	Mean
Emmanuel College	7	5	5	3	2	2	1	1	5	1	1	2	2	1	2	2	4	5	2.8



2004 : Lecturer, Winter School "*Quantum Monte Carlo*", ICTP Trieste.

2006-2014 : Lecturer and Organizer, Summer Schools "*Quantum Monte Carlo and the CASINO program* I-IX", Vallico Sotto, Italy.

2009 : Gave eight-lecture graduate course in the Cavendish Laboratory on quantum dynamical models/quantum trajectory theories.

2012 : Invited instructor, "*Band structure meets many-body theory*" summer school, Vienna, Austria.

2015 : Invited instructor, "*European Workshop on Theoretical Chemistry*", Mariapfarr, Austria.

As a Royal Society Research Fellow I directly supervised Ph.D. students/postdocs in my own Cambridge group, and was indirectly responsible for assisting others through my association with the group of Prof. Richard Needs. Final year undergraduate students sometimes did six-month projects with me, one of which resulted in a publication.

Administrative and management experience

Cavendish Laboratory

1. Member of the staff committee of the Theory of Condensed Matter (TCM) group for almost a decade being thus directly involved with the administration of the group.

2. Conducted interviews with various students looking to work in TCM.

3. Since 2001 organized and chaired weekly 'Electronic Structure Discussion Group' discussion meeting which brought together almost all in Cambridge interested in computer simulation methods of quantum systems (including groups from physics, engineering, chemistry, earth sciences, and biology departments) together with various individuals from institutions in London. Online archive at `vallico.net/casinoqmc/esdg-talk-archive/`.

4. Responsible for maintaining various internal and external websites for the TCM group, where from 1999 I also designed, built, and managed an Italian coffee bar.

Emmanuel College

1. Through College Lectureship became significantly involved in committee work, most notably with the Buildings and Services committee and the Master and Tutors' committee, as well as attending regular meetings of the Governing Body.

2. For three years (2003-2006) was the College internal auditor. Involved attending almost all committee meetings, examining accounts produced by the College Accountant, and writing reports thereon.

3. Acted as a Tutor, with responsibility for the welfare of large numbers of students. This involved regular meetings with the students, and being their first port of call for advice.

4. Conducted annual entrance interviews with large numbers of school students wishing to study Natural Sciences at the university.

5. Evaluated various applications for College Fellowships in physics.

Apuan Alps Centre for Physics

Founder and administrative director of the Apuan Alps Centre for Physics. The centre is situated in a 15th-century monastery in the mountain village of Vallico Sotto in the mountains of northern Tuscany, Italy, about one hour's drive from Pisa. It serves mainly as a venue for international conferences and summer schools of up to 65 people. The institute is largely philanthropic in nature, and costs to visitors are made as small as possible. See `vallico.net/tti/tti.html`.

Research grants and reviewing activity

During over seventeen years in the Cavendish, almost all research funding requirements were met from various rolling grants held collectively by the TCM group, and by the generous research funding provided over nearly a decade in connection with my Royal Society Fel-

lowship (which had to be justified with annual reports). A steady supply of students and postdocs were available 'for free' via association with the group of Prof. Richard Needs.

Have been successful in numerous applications for computer time – both alone and in collaboration – on some of the largest supercomputers available. Recent machines include the Oak Ridge 'Jaguar' machine and its successor 'Titan' through the INCITE program, the Japanese 'K computer', various Blue Gene machines ('Intrepid', 'Mira', 'Vesta') at Argonne National Laboratory, the UK national facilities 'Archer', 'Hector' and 'Hartree' facilities, along with 'Darwin' at the Cambridge High Performance Computing Service.

Obtained a grant from the German Academy of Sciences to host and supervise a postdoc for several years (Martin Korth, now a Junior Professor at the University of Ulm).

In order to run and equip the Apuan Alps Centre for Physics various grants were secured from Psi-k, CCP9, the Royal Society, as well as the Cambridge TCM Group.

For many years I have reviewed a steady stream of scientific articles and grant applications, usually as an expert in quantum Monte Carlo and related techniques.

Selected talks

*Invited presentations marked with *.*

67. Molecular excited states and QMC (Cambridge, U.K., 2014)

66. High-throughput QMC (Vallico Sotto, Italy, 2014)

65*. Quantum Monte Carlo: accuracy, generality, and scalability in the electron correlation problem (Scuola Normale, Pisa, Italy, 2014)

64. Quantum Monte Carlo at the research frontier: useful calculations for big complicated systems (Cambridge, U.K., 2014)

63*. Accurate solutions of the Schrödinger equation for big systems and why they are useful (Oxford University Physics Society, Oxford, U.K., 2013)

62. Some thoughts about Quantum Monte Carlo and molecular dynamics (Cambridge, U.K., 2012)

61*. Quantum Monte Carlo, density functional theory, and many-body physics ("*Band structure meets many-body theory*" summer school, Vienna University, Austria, 2012)

60. Massively-parallel QMC calculations: CPUs, GPUs, and DMC molecular dynamics (Vallico Sotto, Italy, 2012)

59*. The quantum theory of de Broglie and Bohm: twists and turns in quantum foundations (University College London, U.K., 2012)

58. A brief discussion about weak measurements (Cambridge, U.K., 2012)

57. Perfect parallel scaling for quantum Monte Carlo on hundreds of thousands of cores (Cambridge, U.K., 2012)

56*. Art and physics (Royal Academy of Engineering, London, U.K., 2011)

55*. Numerical simulations of the emergence of quantum mechanics (University of Vienna, Austria, 2011)

54*. The quantum theory of de Broglie and Bohm (Oxford University Physics Society, U.K.,

2011)

53*. Further results in out-of-equilibrium quantum physics (Clemson University, U.S.A., 2011)

52. The Coriolis force (Queen Mary University, London, U.K., 2011)

51. Quantum Monte Carlo - a practical solution to the correlation problem in electronic structure calculations (Queen Mary University, London, U.K., 2011)

50*. The quantum theory of de Broglie and Bohm (Chemisch Physikalische Gesellschaft, Vienna, Austria, 2010)

49*. Quantum Monte Carlo - a practical solution to the correlation problem in electronic structure calculations (Vienna University of Technology, Austria, 2010)

48*. A dangerous but enlightening journey (Basil Hiley at 75 Fest, Helsinki, Finland, 2010)

47. Origin of the Born rule (Vallico Sotto, Italy, 2010)

46. 21st-century directions in de Broglie-Bohm theory and beyond - an introduction (Vallico Sotto, Italy, 2010)

45. The magic of moving nodes (Vallico Sotto, Italy, 2010)

44. Dynamical relaxation to quantum equilibrium: introducing the LOUIS code (Cambridge, U.K., 2010)

43. Exchange, antisymmetry, and Pauli repulsion (Cambridge, U.K., 2010)

42*. Quantum Monte Carlo - a practical solution to the correlation problem in electronic structure calculations (Torino, Italy, 2009)

41*. The return of pilot waves, or, why Bohr, Heisenberg, Pauli, Born, Schrödinger, Oppenheimer, Feynman, Wheeler, von Neumann and Einstein were all wrong about quantum mechanics (Cambridge University Physical Society, Cambridge, U.K., 2009) [Note to the worried: the organizers specifically asked me to be (quote) 'amusing and controversial'].

40. Pilot waves, Feynman path integrals, and quantum Monte Carlo (Vallico Sotto, Italy, 2009)

39. Quantum Monte Carlo - is it of any use in quantum chemistry? (Oxford, U.K., 2009)

38. Bohmian metaphysics: the implicate order and other arcana (Cambridge, U.K., 2009)

37. Not even wrong (Cambridge, U.K., 2009)

36. Calculating things with quantum trajectories (Cambridge, U.K., 2009)

35. Nonlocality, relativistic spacetime, and quantum equilibrium (Cambridge, U.K., 2009)

34. The theory of measurement and the origin of randomness (Cambridge, U.K., 2009)

33. Elementary wave mechanics and pilot waves, with nice examples (Cambridge, U.K., 2009)

32. Pilot waves and the classical limit. Derivation and justification of the theory (Cambridge, U.K., 2009)

31. An introduction to pilot-wave theory (Cambridge, U.K., 2009)

30. De Broglie and Bohm's solution to the QM interpretation problem, together with reflections on possible connections with quantum Monte Carlo (Vallico Sotto, Italy, 2008)

29. Another look at pilot wave theory (Cambridge, Italy, 2008)

28*. Recent developments in quantum Monte Carlo: moving the atoms (Thomas Young Centre, London, U.K., 2007)

27. The calculation of expectation values in quantum Monte Carlo (Vallico Sotto, Italy, 2006)

26. Recent progress in quantum Monte Carlo methods (Lyon, France, 2005)

25. Localized orbitals and localized basis sets (Vallico Sotto, Italy, 2005)

24. Quantum Monte Carlo and the metal-insulator transition (Vallico Sotto, Italy, 2005)

23*. Quantum Monte Carlo : practical issues, solid-state applications and the CASINO programme (Trieste, Italy, 2004, three lectures)

22. Coupled quantum Monte Carlo and molecular dynamics (Cambridge, U.K., 2004)

21*. Quantum Monte Carlo and materials physics (Tsukuba, Japan, 2003)

20. The fermion sign problem (Cambridge, U.K., 2003)

19*. Metal-insulator transitions (Melbourne, Australia, 2003)

18*. The quantum Monte Carlo method (Melbourne, Australia, 2003, three lectures)

17. Metal-insulator transitions (Cambridge, U.K., 2001)

16*. The CASINO program : QMC in molecular quantum chemistry and condensed matter physics (Trento, Italy, 2001)

15. An introduction to the quantum Monte Carlo method (Cambridge, U.K., 2000)

14*. The basis set problem in solid-state electronic structure theory (Torino, Italy, 2000)

13*. An introduction to the the quantum Monte Carlo method (Torino, Italy, 2000)

12. Non-collinear spins from first principles (Cambridge, U.K., 2000)

11*. Overview of research in electronic structure theory in the Cambridge TCM group (for international assessment panel, Cambridge, U.K., 2000)

10. Quantum Monte Carlo calculations of crystalline materials (Leicester, U.K., 1999)

9. Quantum Monte Carlo calculations of excited states (Aspen, U.S.A., 1998)

8. Strongly correlated materials in electronic structure theory (Aspen, U.S.A., 1998)

7. Strongly correlated materials in electronic structure theory (Cambridge, U.K., 1997)

6. The transactional interpretation of quantum mechanics (Cambridge, U.K., 1997)

5. The use and optimization of Gaussian basis sets in periodic Hartree–Fock calculations (Torino, Italy, 1995)

4. Equations of state at high pressures and elevated temperatures (Colorado Springs, U.S.A., 1994)

3. The physics of Mott insulators (Birmingham, U.K., 1994)

2. The physics of Mott insulators (Bristol, U.K., 1993)

1. The defect chemistry of lithium niobate (Bristol, U.K., 1993)

Other skills

Computing
Extensive experience of numerical programming and large scale software development on workstations and large parallel machines using Fortran, C, MPI, OpenMP etc. together with various Unix/Linux scripting languages. Specialist in massively parallel applications, with currently active accounts on at least four of the ten most powerful machines in the world. Considerable practical knowledge of GPU programming using CUDA and OpenACC.

Chief developer of the well-known quantum Monte Carlo software package 'CASINO' (which currently has over 600 registered users) and the quantum trajectory code 'LOUIS'.

Experienced in Linux system administration; I run my own extensive network of over 20 machines at the Apuan Alps Centre for Physics (including the web server `vallico.it`).

Experienced in web design. Designer and webmaster of two popular interactive websites featuring my own research: the CASINO QMC site `vallico.net/casinoqmc/` and the CASINO forum `vallico.net/casino-forum` (which now has over 600 subscribers). I also recently designed and built a major new website for the well-known 'Psi-k network' (an EU-funded body active in the promotion and funding of first-principles computational materials science in which I play a minor administrative role). The site at `psi-k.net` became active in April 2015 and is currently successfully hosting many thousands of users.

Languages
English (native); Italian (fluent); French, German (once fluent, now barely adequate through lack of practice)

Hobbies
I manage and curate the Keil Art Bronze gallery in via dei Fossi, Florence, Italy for my wife, the well-known bronze sculptor Sam Keil. Mountain walking. Boogie-woogie piano.

PUBLICATIONS

Citation data (*computed 1st May 2015*)

61 refereed and non-refereed articles (10 with over 50 citations)

Total number of citations: 1899

Total number of citing articles: 1399

Average citations per item: 36.52

h-index: 24

Full list

[61] "Benchmarking the performance of density functional theory and point-charge force fields in their description of sI methane hydrate against diffusion Monte Carlo", S.J. Cox, M.D. Towler, D. Alfè, and A. Michaelides, *J. Chem. Phys*, **140**, 174703 (2014).

[60] "Quantum Monte Carlo and high-level *ab initio* molecular orbital investigation of dissociation channels of the positronic alkali-metal hydrides, [XH;e+] (X=Li, Na, and K)", Y. Yamada, Y. Kita, M. Tachikawa, M.D. Towler, and R.J. Needs, *Eur. Phys. Journal D*, **68**, 63 (2014).

[59] "Assessing the accuracy of quantum Monte Carlo and density functional theory for energetics of water clusters", M.J. Gillan, F.R. Manby, M.D. Towler and D. Alfè, *J. Chem. Phys*, **136**, 244105 (2012).

[58] "Timescales for dynamical relaxation to the Born rule", M.D. Towler, N.J. Russell and A. Valentini, *Proc. Roy. Soc. A* **468**, 990 (2012).

[57] "Petascale computing opens new vistas for quantum Monte Carlo", D. Alfè, M.D. Towler and M.J. Gillan (*Psi-k Newsletter - Highlight of the Month*, February 2011).
`http://psi-k.net/download/highlights/Highlight_103.pdf`

[56] "The lithium-thiophene riddle revisited", M. Korth, S. Grimme and M.D. Towler, *J. Phys. Chem. A* **115**, 11734 (2011).

[55] "*Ab initio* quantum Monte Carlo study of the binding of a positron to alkali-metal hydrides", Y. Kita, R. Maezono, M. Tachikawa, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **135**, 054108 (2011).

[54] "Quantum Monte Carlo computations of phase stability, equations of state, and elasticity of high-pressure silica", K.P. Driver, R.E. Cohen, Z. Wu, B. Militzer, P. López Ríos, M.D. Towler, R.J. Needs, and J.W. Wilkins, *Proc. Nat. Acad. Sci. USA* **107**, 9519 (2010).

[53] "Quantum Monte Carlo, or, how to solve the many-particle Schrödinger equation accurately whilst retaining favourable scaling with system size" M.D. Towler, *Computational Methods for Large Systems* (Wiley, 2010).

[52] "Fundamental high-pressure calibration from all-electron quantum Monte Carlo calculations", K.P. Esler, R.E. Cohen, B. Militzer, J. Kim, R.J. Needs and M.D. Towler, *Phys. Rev. Lett.* **104**, 185702 (2010).

[51] "Benchmark *ab initio* quantum Monte Carlo calculations for small molecules using Slater and Gaussian basis sets", N. Nemec, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **132**, 034111 (2010).

[50] "Continuum variational and diffusion quantum Monte Carlo calculations", R.J. Needs, M.D. Towler, N.D. Drummond and P. López Ríos, *J. Phys.:Cond. Mat.* **22**, 023201 (2010).

[49] "De Broglie-Bohm pilot wave theory and the foundations of quantum mechanics", M.D. Towler (2009). Published online at `www.tcm.phy.cam.ac.uk/~mdt26/pilot_waves.html`.

[48] "*Ab initio* quantum Monte Carlo study of the positronic hydrogen cyanide molecule", Y. Kita, R. Maezono, M. Tachikawa, M.D. Towler, R.J. Needs, *J. Chem. Phys.* **131**, 134310 (2009).

[47] "Quantum Monte Carlo study of porphyrin transition metal complexes", J. Koseki, R. Maezono, M. Tachikawa, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **129**, 085103 (2008).

[46] "Fragmentation method combined with quantum Monte Carlo calculations", R. Maezono, H. Watanabe, S. Tanaka, M.D. Towler and R.J. Needs, *J. Phys. Soc. Jpn.* **76**, 064301 (2007).

[45] "Equation of state and Raman frequency of diamond from quantum Monte Carlo", R. Maezono, A. Ma, M.D. Towler and R.J. Needs, *Phys. Rev. Lett.* **98**, 025701 (2007).

[44] "Quantum Monte Carlo calculations of the dissociation energy of the water dimer", N.A. Benedek, I.K. Snook, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **125**, 104302 (2006).

[43] "Inhomogeneous backflow transformations in quantum Monte Carlo", P. López Ríos, A. Ma, N.D. Drummond, M.D. Towler and R.J. Needs, *Phys. Rev. E.* **74**, 066701 (2006).

[42] "The quantum Monte Carlo method", M.D. Towler, *Phys. Stat. Sol. (b)* **243**, 2573 (2006) .

[41] "Quantum Monte Carlo study of the Ne atom and the Ne^+ ion", N.D. Drummond, P. López Ríos, A. Ma, J.R. Trail, G. Spink, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **124**, 224104 (2006).

[40] "Quantum Monte calculations of the dissociation energies of three-electron hemibonded radical cationic dimers", I.G. Gurtubay, N.D. Drummond, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **124**, 024318 (2006).

[39] "Quantum Monte Carlo calculation of the structural properties and the B1-B2 phase transition of MgO", D. Alfè, M. Alfredsson, J. Brodholt, M.J. Gillan, M.D. Towler and R.J. Needs, *Phys. Rev. B.* **72**, 014114 (2005).

[38] "Scheme for adding electron-nucleus cusps to Gaussian orbitals", A.Ma, N.D. Drummond, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **122**, 224322 (2005).

[37] "All-electron diffusion quantum Monte Carlo calculations for the noble gas atoms He to Xe", A. Ma, N.D. Drummond, M.D. Towler and R.J. Needs, *Phys. Rev. E* **71**, 066704 (2005).

[36] "Diamond and betatin structures of Si studied with quantum Monte Carlo calculations", D. Alfè, M.J. Gillan, M.D. Towler and R.J. Needs, *Phys. Rev. B.* **70**, 214102 (2004).

[35] "Interpretation of Hund's multiplicity rule for the carbon atom" K. Hongo, R. Maezono, Y. Kawazoe, H. Yasuhara, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **121**, 7144 (2004).

[34] "Jastrow correlation factor for atoms, molecules and solids", N.D. Drummond, M.D. Towler and R.J. Needs, *Phys. Rev. B* **70**, 235119 (2004).

[33] "Coulomb finite size effects in quasi-2d systems", B. Wood, W.M.C. Foulkes, M.D. Towler and N.D. Drummond, *J. Phys.: Cond. Mat.* **16**, 891 (2004).

[32] "Diffusion quantum Monte Carlo study of three-dimensional Wigner crystals", N.D. Drummond, Z. Radnai, J.R. Trail, M.D. Towler and R.J. Needs, *Phys. Rev. B* **69**, 085116 (2004).

[31] "Quantum Monte Carlo and the CASINO program : highly accurate total energy calculations for finite and periodic systems", M.D. Towler, (*Psi-k Newsletter - Highlight of the Month*, December 2003).

[30] "Oxygen stripes in $La_{0.5}Ca_{0.5}MnO_3$ from *ab initio* calculations", V. Ferrari, M.D. Towler and P.B. Littlewood, *Phys. Rev. Lett.* **91**, 227202 (2003).

[29] "Stability and aromaticity of B_iN_i rings and fullerenes", J.M. Matxain, J.M. Ugalde, M.D. Towler and R.J. Needs, *J. Phys. Chem. A* **107**, 10004 (2003).

[28] "Quantum Monte Carlo study of sodium", R. Maezono, M.D. Towler, Y. Lee and R.J. Needs, *Phys. Rev. B* **68**, 165103 (2003).

[27["Unrestricted Hartree-Fock theory of Wigner crystals", J.R. Trail, M.D. Towler and R.J. Needs, *Phys. Rev. B* **68**, 045107 (2003).

[26] "Electronic structure of *p*-type conducting transparent oxides", J. Robertson, P.W. Peacock, M.D. Towler and R.J. Needs, *Thin Solid Films* **411**, 96 (2002).

[25] "Quantum Monte Carlo calculations for excited electronic states", R.J. Needs, A.R. Porter, and M.D. Towler, "*Recent Advances in Quantum Monte Carlo Methods, II*", ed. W.A. Lester, S. Rothstein and S. Tanaka (World Scientific, 2002).

[24] "The diffusion quantum Monte Carlo method: designing trial wave functions for NiO", R.J. Needs and M.D. Towler, *Proceedings of the 11th International Conference on Recent Progress in Many-Body Theories*, Eds. R.F. Bishop and N.R. Walet (World Scientific, 2001).

[23] "The CASINO program : quantum Monte Carlo in molecular quantum chemistry and condensed matter physics", M.D. Towler, *Quantum Monte Carlo: Recent Advances and Common Problems in Condensed Matter and Field Theory* (ETS, Pisa, 2001).

[22] "Quantum Monte Carlo calculations for ground and excited states", R.J. Needs, P.R. C. Kent, A.R. Porter, M.D. Towler, and G. Rajagopal, *Int. J. Quant. Chem.* **86**, 218 (2001).

[21] "Excitons in small hydrogenated silicon clusters", A.R. Porter, M.D. Towler and R.J. Needs, *Phys. Rev. B* **64**, 035320 (2001).

[20] "Electronic excited-state wave functions for quantum Monte Carlo: application to silane and methane", A.R. Porter, O.K. Al-Mushadani, M.D. Towler and R.J. Needs, *J. Chem. Phys.* **114**, 7795 (2001).

[19] "Carbon clusters near the crossover to fullerene stability", P.R.C. Kent, M.D. Towler, R.J. Needs and G. Rajagopal, *Phys. Rev. B* **62**, 15394 (2000).

[18] "Pseudopotentials for correlated-electron calculations", Y. Lee, P.R.C. Kent, M.D. Towler, R.J. Needs and G. Rajagopal, *Phys. Rev. B* **62**, 13347 (2000).

[17] "Minimum principles and level splittings in quantum Monte Carlo excitation spectra: application to diamond", M.D. Towler, R.Q. Hood and R.J. Needs, *Phys. Rev. B* **62**, 2300 (2000).

[16] "Muonium as a hydrogen analogue in silicon and germanium; quantum effects and hyperfine parameters", A.R. Porter, M.D. Towler and R.J. Needs, *Phys. Rev. B* **60**, 13534 (1999).

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