

List of publications

Mike Towler

- [1] “Modelling explosives”, N.L. Allan, M.D. Towler, M. Braithwaite, D.L. Cooper and W.C. Mackrodt, in *CCP5 Information Quarterly for Computer Simulation of Condensed Phases*, ed. W. Smith, **36** (1992).
- [2] “*Ab initio* Hartree-Fock calculations of CaO, VO, MnO and NiO”, W.C. Mackrodt, N.M. Harrison, V.R. Saunders, N.L. Allan, M.D. Towler, E. Aprà and R. Dovesi, *Phil. Mag. A* **68**, 653 (1993).
- [3] “Quantum-mechanical and empirical approaches to solid state theory”, M.D. Towler, Ph.D. thesis (University of Bristol, 1994).
- [4] “Calculated pressure-induced phase transition in MgF₂”, N.L. Allan, R.I. Hines, M.D. Towler and W.C. Mackrodt, *J. Chem. Phys.* **100**, 4710 (1994).
- [5] “*Ab initio* study of MnO and NiO”, M.D. Towler, N.L. Allan, N.M. Harrison, V.R. Saunders, W.C. Mackrodt and E. Aprà, *Phys. Rev. B* **50**, 5041 (1994).
- [6] “Equations of state for polar solids at high pressures and elevated temperatures”, M.D. Towler, R.I. Hines, N.L. Allan, M. Braithwaite and W.C. Mackrodt, in *Proc. AIRAPT/APS Topical conference, High Pressure Science and Technology*, ed. S.C. Schmidt (1994).
- [7] “Localized electron behaviour within band theory: a Hartree-Fock description of M_xMg_{1-x}O (M=Mn,Ni)”, M.D. Towler, N.L. Allan, N.M. Harrison, V.R. Saunders and W.C. Mackrodt, *J. Phys.: Condens. Matt.* **7**, 6231 (1995).
- [8] “*Ab initio* study of the surface and interfacial properties of a layered MgO/NiO film”, M.D. Towler, N.M. Harrison and M.I. McCarthy, *Phys. Rev. B* **52**, 5375 (1995).
- [9] “Magnetic interactions and the cooperative Jahn-Teller effect in KCuF₃”, M.D. Towler, R. Dovesi and V.R. Saunders, *Phys. Rev. B* **52**, 10150 (1995).
- [10] “The use and optimization of Gaussian basis sets in periodic Hartree-Fock calculations”, M.D. Towler, *Proceedings of HCM Network School “Hartree-Fock theory of the electronic structure of solids”*, ed. C. Pisani, (1995).
- [11] “Cluster and supercell calculations of carbon-doped silicon”, R. Orlando, P. Azavant, M.D. Towler, R. Dovesi and C. Roetti, *J. Phys.: Condens. Matt.* **8**, 1223 (1996).
- [12] “Direct evidence of O(p) holes in Li-doped NiO from Hartree-Fock calculations”, W.C. Mackrodt, N.M. Harrison, V.R. Saunders, N.L. Allan and M.D. Towler, *Chem. Phys. Lett.* **250**, 66 (1996).

- [13] “Density functional theory in periodic systems using local Gaussian basis sets”, M.D. Towler, M. Causà, and A. Zupan, *Comp. Phys. Commun.* **98**, 181-205 (1996).
- [14] “Quantum Monte Carlo calculations of the one-body density matrix and excitation energies of silicon”, P.R.C. Kent, R.Q. Hood, M.D. Towler, R.J. Needs and G. Rajagopal, *Phys. Rev. B* **57**, 15293 (1998).
- [15] “Quantum Monte Carlo simulations of real solids”, W.M.C. Foulkes, M. Nekovee, R.L. Gaudoin, M.L. Stedman, R.J. Needs, R.Q. Hood, G. Rajagopal, M.D. Towler, P.R.C. Kent, Y. Lee, W.K. Leung, A.R. Porter and S.J. Breuer., *High Performance Computing*, edited by R.J. Allan, M.F. Guest, A.D. Simpson, D.S. Henty, and D.A. Nicole (Plenum, 1998).
- [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).
- [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).
- [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).
- [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).
- [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).
- [21] “Excitons in small hydrogenated silicon clusters”, A.R. Porter, M.D. Towler and R.J. Needs, *Phys. Rev. B* **64**, 035320 (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).
- [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).
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- [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).
- [27] “Unrestricted Hartree-Fock theory of Wigner crystals”, J.R. Trail, M.D. Towler and R.J. Needs, *Phys. Rev. B* **68**, 045107 (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).
- [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).
- [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).
- [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).
- [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).
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- [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).
- [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).
- [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).

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- [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).
- [42] “The quantum Monte Carlo method”, M.D. Towler, *Phys. Stat. Sol. (b)* **243**, 2573 (2006) .
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- [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).
- [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).
- [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).
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- [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).
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- [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).
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- [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).
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- [56] “The lithium-thiophene riddle revisited”, M. Korth, S. Grimme and M.D. Towler, *J. Chem. Phys.* **115**, 11734 (2011).
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- [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).
- [59] “Linear scaling with number of cores for diffusion Monte Carlo calculations on petascale computers”, M.D. Towler (submitted to *Comp. Phys. Commun.*, 2011).
- [60] “Dynamical relaxation to quantum equilibrium in three dimensions”, M.D. Towler and A. Valentini (in preparation, 2011).
- [61] “Energetics of water clusters: assessing the accuracy of quantum Monte Carlo and density functional theory”, M.J. Gillan, F.R. Manby, M.D. Towler and D. Alfè (to be submitted to *J. Chem. Phys.*, 2012).

Citation data

61 articles (9 with over 50 citations)

Total number of citations: 1314

Total number of citing articles: 989

Average citations per item: 23.89

h-index: 20