# Richard J Wheatley

List of Publications by Year
in descending order



| 86 | 2,342 | 249298 | 263392 |
|---|---|---|---|
| papers | citations | 26 h-index | 45 g-index |

| 89 | 89 | 89 | 1887 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Gaussian process models of potential energy surfaces with boundary optimization. Journal of Chemical Physics, 2021, 155, 144106. | 1.2 | 8 |
| 2 | Enhanced doping effects of multielement on anisotropic thermal expansion in ZrO<sub>2</sub> with new compositions. Journal of the American Ceramic Society, 2020, 103, 5881-5890. | 1.9 | 17 |
| 3 | Cluster integrals and virial coefficients for realistic molecular models. Physical Review E, 2020, 101, 051301. | 0.8 | 9 |
| 4 | Simulation of the Raman spectroscopy of multi-layered carbon nanomaterials. Physical Chemistry Chemical Physics, 2018, 20, 28001-28010. | 1.3 | 8 |
| 5 | Active learning in Gaussian process interpolation of potential energy surfaces. Journal of Chemical Physics, 2018, 149, 174114. | 1.2 | 44 |
| 6 | An empirical force field for the simulation of the vibrational spectroscopy of carbon nanomaterials. Carbon, 2017, 113, 299-308. | 5.4 | 12 |
| 7 | Interpolation of intermolecular potentials using Gaussian processes. Journal of Chemical Physics, 2017, 147, 161706. | 1.2 | 38 |
| 8 | An Atomistic-Scale Study for Thermal Conductivity and Thermochemical Compatibility in (DyY)Zr2O7 Combining an Experimental Approach with Theoretical Calculation. Scientific Reports, 2016, 6, 21232. | 1.6 | 3 |
| 9 | Molecular simulation of the thermophysical properties and phase behaviour of impure CO2 relevant to CCS. Faraday Discussions, 2016, 192, 415-436. | 1.6 | 10 |
| 10 | Calculation of high-order virial coefficients for the square-well potential. Physical Review E, 2016, 94, 013301. | 0.8 | 8 |
| 11 | Reverse energy partitioningâ€"An efficient algorithm for computing the density of states, partition functions, and free energy of solids. Journal of Chemical Physics, 2016, 145, 084116. | 1.2 | 6 |
| 12 | Investigation of La3+ Doped Yb2Sn2O7 as new thermal barrier materials. Materials and Design, 2015, 85, 423-430. | 3.3 | 11 |
| 13 | Density of States Partitioning Method for Calculating the Free Energy of Solids. Journal of Chemical Theory and Computation, 2013, 9, 165-171. | 2.3 | 17 |
| 14 | Calculation of High-Order Virial Coefficients with Applications to Hard and Soft Spheres. Physical Review Letters, 2013, 110, 200601. | 2.9 | 77 |
| 15 | Covalent bond orders and atomic anisotropies from iterated stockholder atoms. Physical Chemistry Chemical Physics, 2012, 14, 2087. | 1.3 | 16 |
| 16 | Calculation of Partition Functions and Free Energies of a Binary Mixture Using the Energy Partitioning Method: Application to Carbon Dioxide and Methane. Journal of Physical Chemistry B, 2012, 116, 4535-4542. | 1.2 | 21 |
| 17 | Molecular simulation of the binary mixture of 1â€"1â€"1â€"2â€"tetrafluoroethane and carbon dioxide. Physical Chemistry Chemical Physics, 2011, 13, 15708. | 1.3 | 4 |
| 18 | Intermolecular potential energy surface and second virial coefficients for the waterâ€"CO2 dimer. Journal of Chemical Physics, 2011, 134, 134309. | 1.2 | 29 |

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|---|---|---|---|
| 19 | Rapid calculation of partition functions and free energies of fluids. Journal of Chemical Physics, 2011, 135, 174105. | 1.2 | 27 |
| 20 | First principles predictions of thermophysical properties of refrigerant mixtures. Journal of Chemical Physics, 2011, 134, 114518. | 1.2 | 5 |
| 21 | First principles models of the interactions of methane and carbon dioxide. Fluid Phase Equilibria, 2010, 290, 48-54. | 1.4 | 18 |
| 22 | Gibbs Ensemble Monte Carlo Simulations of Binary Mixtures of Methane, Difluoromethane, and Carbon Dioxide. Journal of Physical Chemistry B, 2010, 114, 3879-3886. | 1.2 | 21 |
| 23 | Microscopic structure of liquid 1-1-1-2-tetrafluoroethane (R134a) from Monte Carlo simulation. Physical Chemistry Chemical Physics, 2010, 12, 13266. | 1.3 | 11 |
| 24 | Atomic Polarizabilities and Dispersion Energy Coefficients. , 2009, , . | | 0 |
| 25 | Intermolecular potential energy surface and second virial coefficients for the nonrigid water-CO dimer. Journal of Chemical Physics, 2009, 131, 154305. | 1.2 | 24 |
| 26 | Additive and nonadditive models of vapor-liquid equilibrium in CO2 from first principles. Journal of Chemical Physics, 2009, 130, 034110. | 1.2 | 33 |
| 27 | Intermolecular potential and ab initio spectroscopy of the Neâ€“HF complex. Chemical Physics Letters, 2009, 468, 290-293. | 1.2 | 1 |
| 28 | Atomic charge densities generated using an iterative stockholder procedure. Journal of Chemical Physics, 2009, 131, 144101. | 1.2 | 83 |
| 29 | Timeâ€dependent coupledâ€cluster calculations of polarizabilities and dispersion energy coefficients. Journal of Computational Chemistry, 2008, 29, 445-450. | 1.5 | 25 |
| 30 | The Specific Work of Flow as a Criterion for Orientation in Polymer Crystallization. Macromolecules, 2008, 41, 1901-1904. | 2.2 | 185 |
| 31 | Redefining the atom: atomic charge densities produced by an iterative stockholder approach. Chemical Communications, 2008, , 5909. | 2.2 | 111 |
| 32 | Local polarizabilities and dispersion energy coefficients. Molecular Physics, 2008, 106, 1545-1556. | 0.8 | 18 |
| 33 | The water-oxygen dimer: First-principles calculation of an extrapolated potential energy surface and second virial coefficients. Journal of Chemical Physics, 2007, 127, 074303. | 1.2 | 18 |
| 34 | Blueshift and intramolecular tunneling of NH3 umbrella mode in Hen4 clusters. Journal of Chemical Physics, 2007, 127, 194303. | 1.2 | 14 |
| 35 | First-Principles Calculation of Local Atomic Polarizabilities. Journal of Physical Chemistry A, 2007, 111, 11141-11146. | 1.1 | 34 |
| 36 | Intermolecular potential and second virial coefficient of the water-nitrogen complex. Journal of Chemical Physics, 2007, 126, 094305. | 1.2 | 44 |

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| 37 | Calculating intermolecular potentials with SIMPER: the waterâ€“nitrogen and waterâ€“oxygen interactions, dispersion energy coefficients, and preliminary results for larger molecules. International Reviews in Physical Chemistry, 2007, 26, 449-485. | 0.9 | 8 |
| 38 | A reliable new three-dimensional potential energy surface for H2â€“Kr. Journal of Chemical Physics, 2005, 122, 084321. | 1.2 | 41 |
| 39 | Density functional theory of liquid crystals and surface anchoring. Physical Review E, 2005, 72, 061706. | 0.8 | 16 |
| 40 | Electronic spectroscopy of the deuterated isotopomers of the NOâˆ™methane molecular complex. Journal of Chemical Physics, 2005, 123, 204305. | 1.2 | 14 |
| 41 | Inverse Power Potentials:Â Virial Coefficients and a General Equation of State. Journal of Physical Chemistry B, 2005, 109, 7463-7467. | 1.2 | 22 |
| 42 | Density profile and order parameter of a hard ellipsoidal fluid confined to a slit. Journal of Physics Condensed Matter, 2005, 17, 5625-5634. | 0.7 | 17 |
| 43 | Extrapolation methods and scaled perturbation theory for determining intermolecular potential energy surfaces. International Journal of Quantum Chemistry, 2004, 96, 537-546. | 1.0 | 5 |
| 44 | Ab initio spectroscopy of Van der Waals molecules: a comparison of three different theoretical methods applied to NeHF and NeDF. Chemical Physics Letters, 2004, 393, 70-75. | 1.2 | 1 |
| 45 | Intermolecular potential energy extrapolation method for weakly bound systems: Ar2, Arâ€“H2and Arâ€“HF dimers. Molecular Physics, 2004, 102, 567-577. | 0.8 | 8 |
| 46 | Intermolecular potentials from supermolecule and monomer calculations. International Reviews in Physical Chemistry, 2004, 23, 151-185. | 0.9 | 22 |
| 47 | Intermolecular potential and second virial coefficient of the waterâ€“hydrogen complex. Journal of Chemical Physics, 2004, 120, 710-720. | 1.2 | 82 |
| 48 | An environmental pseudopotential approach to molecular interactions: Implementation in MOLPRO. Journal of Computational Chemistry, 2003, 24, 2075-2082. | 1.5 | 13 |
| 49 | Atomic representation of the dispersion interaction energy. Physical Chemistry Chemical Physics, 2003, 5, 801-807. | 1.3 | 8 |
| 50 | Intermolecular potential and second virial coefficient of the waterâ€“helium complex. Journal of Chemical Physics, 2002, 116, 1397-1405. | 1.2 | 59 |
| 51 | Intermolecular potentials and second virial coefficients of the waterâ€“neon and waterâ€“argon complexes. Journal of Chemical Physics, 2002, 117, 7169-7179. | 1.2 | 62 |
| 52 | Extrapolation of intermolecular interaction energies in weakly bound Van der Waals complexes. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 391-397. | 0.1 | 6 |
| 53 | Scaled perturbation theory for weak intermolecular forces: the helium dimer. Computational and Theoretical Chemistry, 2002, 591, 67-76. | 1.5 | 10 |
| 54 | Short-Range Contributions to the Polarization of Cations. Journal of Physical Chemistry A, 2001, 105, 4136-4142. | 1.1 | 26 |

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|---|---|---|---|
| 55 | Overlap-model and ab initio cluster calculations of ion properties in distorted environments. Chemical Physics Letters, 2001, 333, 403-412. | 1.2 | 35 |
| 56 | Intermolecular potential for the interaction of helium with ammonia. Journal of Chemical Physics, 2001, 114, 8836-8843. | 1.2 | 38 |
| 57 | Application of the overlap model to calculating correlated exchange energies. Chemical Physics Letters, 2000, 326, 263-268. | 1.2 | 20 |
| 58 | Flexible multipole models for hydrogen fluoride. Physical Chemistry Chemical Physics, 2000, 2, 1631-1638. | 1.3 | 2 |
| 59 | Using Computer Assisted Learning to Teach Molecular Reaction Dynamics. Journal of Chemical Education, 2000, 77, 407. | 1.1 | 5 |
| 60 | On the virial series for hard-sphere mixtures. Journal of Chemical Physics, 1999, 111, 5455-5460. | 1.2 | 20 |
| 61 | The sixth virial coefficient of hard disc mixtures. Molecular Physics, 1999, 96, 1805-1811. | 0.8 | 11 |
| 62 | On the non-additive second-order Coulomb energy for H<sub>3</sub> in C<sub>2v</sub> geometries. Molecular Physics, 1999, 96, 53-60. | 0.8 | 1 |
| 63 | Overlap model and ab initio cluster calculations of polarisabilities of ions in solids. Chemical Physics Letters, 1999, 314, 158-167. | 1.2 | 19 |
| 64 | The sixth virial coefficient of hard disc mixtures. , 1999, . | | 1 |
| 65 | An overlap model for exchange-induction: application to alkali halides. Chemical Physics Letters, 1998, 294, 487-492. | 1.2 | 15 |
| 66 | RESEARCH NOTE Fifth virial coefficient of hard sphere mixtures. Molecular Physics, 1998, 94, 877-879. | 0.8 | 8 |
| 67 | Structure and vibrational spectra of methanol clusters from a new potential model. Journal of Chemical Physics, 1998, 108, 20-32. | 1.2 | 101 |
| 68 | Use of molecular overlap to predict intermolecular repulsion in N... H-O hydrogen bonds. Molecular Physics, 1998, 95, 525-537. | 0.8 | 4 |
| 69 | Vibrational predissociation spectra of size selected hydrazine clusters: Experiment and calculations. Journal of Chemical Physics, 1997, 106, 6806-6812. | 1.2 | 17 |
| 70 | A new intermolecular potential for hydrazine clusters: Structures and spectra. Journal of Chemical Physics, 1997, 106, 6795-6805. | 1.2 | 19 |
| 71 | The intermolecular potential energy surface for CO2â€“Ar: Fitting to highâ€resolution spectroscopy of Van der Waals complexes and second virial coefficients. Journal of Chemical Physics, 1996, 105, 9130-9140. | 1.2 | 80 |
| 72 | Dispersion and induction energy damping functions, and their scale with interspecies distance, for the interaction of Hâ¯ with H, He and Li atoms. Chemical Physics, 1996, 203, 209-221. | 0.9 | 2 |

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|---|---|---|---|
| 73 | A reliable new potential energy surface for H2â€“Ar. Journal of Chemical Physics, 1996, 105, 2639-2653. | 1.2 | 71 |
| 74 | The solvation of sodium ions in water clusters: intermolecular potentials for Na+-H2O and H2O-H2O. Molecular Physics, 1996, 87, 1083-1116. | 0.8 | 28 |
| 75 | The solvation of sodium ions in water clusters: intermolecular potentials for Na+-H2O and H2O-H2O. Molecular Physics, 1996, 87, 1083-1116. | 0.8 | 8 |
| 76 | A systematic model potential for Li+-H2O. Molecular Physics, 1995, 84, 879-898. | 0.8 | 11 |
| 77 | The non-additive exchange energies of H3and He3. Molecular Physics, 1995, 84, 899-910. | 0.8 | 5 |
| 78 | Induction and dispersion damping functions, and their relative scale with interspecies distance, for (H+, He+, Li+)-(H, He, Li) interactions. Chemical Physics, 1994, 179, 341-364. | 0.9 | 19 |
| 79 | Gaussian multipoles in practice: Electrostatic energies for intermolecular potentials. Journal of Computational Chemistry, 1994, 15, 1187-1198. | 1.5 | 77 |
| 80 | A new distributed multipole procedure for linear molecules. Chemical Physics Letters, 1993, 208, 159-166. | 1.2 | 7 |
| 81 | Dispersion energy damping functions, and their relative scale with interatomic separation, for (H, He,) Tj ETQq1 1 0.784314 rgBT /Ove | 0.8 | 37 |
| 82 | On the relationship between first-order exchange and Coulomb interaction energies for closed shell atoms and molecules. Molecular Physics, 1993, 79, 253-275. | 0.8 | 25 |
| 83 | Gaussian multipole functions for describing molecular charge distributions. Molecular Physics, 1993, 79, 597-610. | 0.8 | 37 |
| 84 | A systematic intermolecular potential method applied to chlorine. Molecular Physics, 1990, 71, 1381-1404. | 0.8 | 56 |
| 85 | An overlap model for estimating the anisotropy of repulsion. Molecular Physics, 1990, 69, 507-533. | 0.8 | 103 |
| 86 | Machine learning for non-additive intermolecular potentials: quantum chemistry to first-principles predictions. Chemical Communications, 0, , . | 2.2 | 7 |