# Andrew C Simmonett

List of Publications by Year
in descending order

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|---|---|---|---|
| 62<br>papers | 8,328<br>citations | 218677<br>26<br>h-index | 118850<br>62<br>g-index |
| 70<br>all docs | 70<br>docs citations | 70<br>times ranked | 9403<br>citing authors |

| # | Article | IF | Citations |
|---|---------|-----|-----------|
| 1 | A simplified charge projection scheme for long-range electrostatics in *ab initio* QM/MM calculations. Journal of Chemical Physics, 2021, 154, 024115. | 3.0 | 18 |
| 2 | Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. Journal of Chemical Theory and Computation, 2021, 17, 1562-1580. | 5.3 | 39 |
| 3 | A compression strategy for particle mesh Ewald theory. Journal of Chemical Physics, 2021, 154, 054112. | 3.0 | 18 |
| 4 | Analytical Hessians for Ewald and particle mesh Ewald electrostatics. Journal of Chemical Physics, 2021, 154, 104101. | 3.0 | 8 |
| 5 | Thermodynamic Decomposition of Solvation Free Energies with Particle Mesh Ewald and Long-Range Lennard-Jones Interactions in Grid Inhomogeneous Solvation Theory. Journal of Chemical Theory and Computation, 2021, 17, 2714-2724. | 5.3 | 19 |
| 6 | The Extended Eighth‐Shell method for periodic boundary conditions with rotational symmetry. Journal of Computational Chemistry, 2021, 42, 1373-1383. | 3.3 | 2 |
| 7 | Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801. | 3.0 | 15 |
| 8 | PSI4 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108. | 3.0 | 440 |
| 9 | Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. Journal of Chemical Theory and Computation, 2019, 15, 3854-3867. | 5.3 | 25 |
| 10 | Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. Journal of Chemical Theory and Computation, 2018, 14, 948-958. | 5.3 | 50 |
| 11 | Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511. | 5.3 | 106 |
| 12 | An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. Journal of Chemical Theory and Computation, 2017, 13, 679-695. | 5.3 | 19 |
| 13 | Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197. | 5.3 | 961 |
| 14 | Mapping the Drude polarizable force field onto a multipole and induced dipole model. Journal of Chemical Physics, 2017, 147, 161702. | 3.0 | 42 |
| 15 | OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659. | 3.2 | 1,561 |
| 16 | An empirical extrapolation scheme for efficient treatment of induced dipoles. Journal of Chemical Physics, 2016, 145, 164101. | 3.0 | 27 |
| 17 | Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK a corrections. Journal of Computer-Aided Molecular Design, 2016, 30, 1087-1100. | 2.9 | 27 |
| 18 | An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. Bioorganic and Medicinal Chemistry, 2016, 24, 4988-4997. | 3.0 | 15 |

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| 19 | Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 989-1006. | 2.9 | 24 |
| 20 | Molecular Multipole Potential Energy Functions for Water. Journal of Physical Chemistry B, 2016, 120, 1833-1842. | 2.6 | 10 |
| 21 | Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. Journal of Chemical Theory and Computation, 2016, 12, 332-344. | 5.3 | 42 |
| 22 | Efficient treatment of induced dipoles. Journal of Chemical Physics, 2015, 143, 074115. | 3.0 | 38 |
| 23 | Numerical Study on the Partitioning of the Molecular Polarizability into Fluctuating Charge and Induced Atomic Dipole Contributions. Journal of Physical Chemistry A, 2015, 119, 5865-5882. | 2.5 | 44 |
| 24 | Quantum Mechanical Molecular Mechanical Calculations using AMOEBA Force Fields. Biophysical Journal, 2015, 108, 158a. | 0.5 | 1 |
| 25 | An efficient algorithm for multipole energies and derivatives based on spherical harmonics and extensions to particle mesh Ewald. Journal of Chemical Physics, 2014, 140, 184101. | 3.0 | 43 |
| 26 | New Potential Energy Surface Features for the Li + HF → LiF + H Reaction. Journal of Physical Chemistry A, 2013, 117, 10027-10033. | 2.5 | 10 |
| 27 | Density cumulant functional theory: The DC-12 method, an improved description of the one-particle density matrix. Journal of Chemical Physics, 2013, 138, 024107. | 3.0 | 17 |
| 28 | Anharmonic vibrational analyses for the 1-silacyclopropenylidene molecule and its three isomers. Molecular Physics, 2012, 110, 783-800. | 1.7 | 5 |
| 29 | Analytic gradients for density cumulant functional theory: The DCFT-06 model. Journal of Chemical Physics, 2012, 137, 054105. | 3.0 | 18 |
| 30 | 1-Germavinylidene (Geâ•CH$_2$), Germyne (HGeCH), and 2-Germavinylidene (H$_2$Geâ•C) Molecules and Isomerization Reactions among Them: Anharmonic Rovibrational Analyses. Journal of Physical Chemistry A, 2012, 116, 4578-4589. | 2.5 | 7 |
| 31 | Characterization of the *t*-Butyl Radical and Its Elusive Anion. Journal of Chemical Theory and Computation, 2012, 8, 4323-4329. | 5.3 | 5 |
| 32 | Psi4: an openâ€source *ab initio* electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565. | 14.6 | 838 |
| 33 | Fundamental vibrational frequencies and spectroscopic constants for the methylperoxyl radical, $CH_3O_2$, and related isotopologues $^{13}CH_3OO$, $CH_3$ $^{18}O^{18}O$, and $CD_3OO$. Molecular Physics, 2012, 110, 2419-2427. | 1.7 | 13 |
| 34 | The Beryllium Pentamer: Trailing an Uneven Sequence of Dissociation Energies. ChemPhysChem, 2012, 13, 1255-1260. | 2.1 | 5 |
| 35 | The benzene+OH potential energy surface: intermediates and transition states. Physical Chemistry Chemical Physics, 2011, 13, 2214-2221. | 2.8 | 28 |
| 36 | Combustion Chemistry: Important Features of the $C_3H_5$ Potential Energy Surface, Including Allyl Radical, Propargyl + $H_2$, Allene + H, and Eight Transition States. Journal of Physical Chemistry A, 2011, 115, 14209-14214. | 2.5 | 25 |

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| 37 | Toward Functional Ni-SOD Biomimetics: Achieving a Structural/Electronic Correlation with Redox Dynamics. Inorganic Chemistry, 2011, 50, 9216-9218. | 4.0 | 32 |
| 38 | From acetylene complexes to vinylidene structures: The $GeC_2H_2$ system. Journal of Computational Chemistry, 2011, 32, 15-22. | 3.3 | 3 |
| 39 | Silacyclopropenylidene and Its Most Important $SiC_2H_2$ Isomers. Journal of Physical Chemistry C, 2010, 114, 5447-5457. | 3.1 | 13 |
| 40 | Reactions between Resonance-Stabilized Radicals: Propargyl + Allyl. Journal of Physical Chemistry A, 2010, 114, 4881-4890. | 2.5 | 84 |
| 41 | Low-Lying Triplet States of Diphosphene and Diphosphinylidene. Journal of Physical Chemistry A, 2010, 114, 10850-10856. | 2.5 | 7 |
| 42 | Characterization of the BNNO Radical. Journal of Chemical Theory and Computation, 2010, 6, 1915-1923. | 5.3 | 1 |
| 43 | Exploring the Effects of H-Bonding in Synthetic Analogues of Nickel Superoxide Dismutase (Ni-SOD): Experimental and Theoretical Implications for Protection of the Niâ˜ SCys Bond. Inorganic Chemistry, 2010, 49, 7080-7096. | 4.0 | 43 |
| 44 | Anharmonic Vibrational Analysis for the Propadienylidene Molecule (H2Câ•Câ•C:). Journal of Chemical Theory and Computation, 2010, 6, 3122-3130. | 5.3 | 4 |
| 45 | Density cumulant functional theory: First implementation and benchmark results for the DCFT-06 model. Journal of Chemical Physics, 2010, 133, 174122. | 3.0 | 26 |
| 46 | Diphosphene and Diphosphinylidene. Journal of Physical Chemistry A, 2009, 113, 13227-13236. | 2.5 | 14 |
| 47 | Structures and Energetics of H6+ Clusters. Journal of Physical Chemistry A, 2009, 113, 13608-13620. | 2.5 | 6 |
| 48 | Water Dimer Radical Cation: Structures, Vibrational Frequencies, and Energetics. Journal of Physical Chemistry A, 2009, 113, 13779-13789. | 2.5 | 63 |
| 49 | Barrier To Linearity and Anharmonic Force Field of the Ketenyl Radical. Journal of Physical Chemistry A, 2009, 113, 11643-11650. | 2.5 | 12 |
| 50 | Enthalpy of formation and anharmonic force field of diacetylene. Journal of Chemical Physics, 2009, 130, 044301. | 3.0 | 41 |
| 51 | A companion perturbation theory for state-specific multireference coupled cluster methods. Physical Chemistry Chemical Physics, 2009, 11, 4728. | 2.8 | 65 |
| 52 | Infrared signatures of the NCCO radical. Physical Chemistry Chemical Physics, 2009, 11, 10385. | 2.8 | 13 |
| 53 | Capture of hydroxymethylene and its fast disappearance through tunnelling. Nature, 2008, 453, 906-909. | 27.8 | 264 |
| 54 | Anchoring the Absolute Proton Affinity Scale. Journal of Chemical Theory and Computation, 2008, 4, 1220-1229. | 5.3 | 42 |

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| 55 | $\pi$ and $\sigma$-Phenylethynyl Radicals and Their Isomers <i>o-</i>, <i>m-</i>, and <i>p-</i>Ethynylphenyl:‰ Structures, Energetics, and Electron Affinities. Journal of Physical Chemistry A, 2008, 112, 2838-2845. | 2.5 | 5 |
| 56 | Triple excitations in state-specific multireference coupled cluster theory: Application of Mk-MRCCSDT and Mk-MRCCSDT-n methods to model systems. Journal of Chemical Physics, 2008, 128, 124104. | 3.0 | 123 |
| 57 | In search of definitive signatures of the elusive NCCO radical. Journal of Chemical Physics, 2007, 127, 014306. | 3.0 | 19 |
| 58 | Renner–Teller Bending Frequencies of the $\tilde{A}$ $^2\Pi$ State of OCS+. Journal of Physical Chemistry A, 2007, 111, 4551-4555. | 2.5 | 5 |
| 59 | Popular Theoretical Methods Predict Benzene and Arenes To Be Nonplanar. Journal of the American Chemical Society, 2006, 128, 9342-9343. | 13.7 | 238 |
| 60 | Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191. | 2.8 | 2,597 |
| 61 | An optimal point-charge model for molecular electrostatic potentials. Molecular Physics, 2005, 103, 2789-2793. | 1.7 | 15 |
| 62 | The Vinyl Radical and Fluorinated Vinyl Radicals, C2H3-nFn (n = 0–3), and Corresponding Anions:‰ Comparison with the Isoelectronic Complexes [X·Â·Â·YC‰¡CZ]-. Journal of Physical Chemistry A, 2004, 108, 1608-1615. | 2.5 | 12 |