Edward G Hohenstein

List of Publications by Year
in descending order

72 papers	11,050 citations	66234 42 h-index	85405 71 g-index
77 all docs	77 docs citations	77 times ranked	9779 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	2.3	961
3	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	6.2	838
4	Assessment of the Performance of the M05â^'2X and M06â^'2X Exchange-Correlation Functionals for Noncovalent Interactions in Biomolecules. Journal of Chemical Theory and Computation, 2008, 4, 1996-2000.	2.3	685
5	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
6	Assessment of the Performance of DFT and DFT-D Methods for Describing Distance Dependence of Hydrogen-Bonded Interactions. Journal of Chemical Theory and Computation, 2011, 7, 88-96.	2.3	388
7	An Assessment of Theoretical Methods for Nonbonded Interactions: Comparison to Complete Basis Set Limit Coupled-Cluster Potential Energy Curves for the Benzene Dimer, the Methane Dimer, Benzeneâ^'Methane, and Benzeneâ^'H₂S. Journal of Physical Chemistry A, 2009, 113, 10146-10159.	1.1	369
8	Wavefunction methods for noncovalent interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 304-326.	6.2	345
9	Effects of Heteroatoms on Aromatic Ï€â^'Ï€ Interactions: Benzeneâ^'Pyridine and Pyridine Dimer. Journal of Physical Chemistry A, 2009, 113, 878-886.	1.1	328
10	Basis set consistent revision of the S22 test set of noncovalent interaction energies. Journal of Chemical Physics, 2010, 132, 144104.	1.2	309
11	Density fitting and Cholesky decomposition approximations in symmetry-adapted perturbation theory: Implementation and application to probe the nature of Ï€-Ï€ interactions in linear acenes. Journal of Chemical Physics, 2010, 132, .	1.2	266
12	Density fitting of intramonomer correlation effects in symmetry-adapted perturbation theory. Journal of Chemical Physics, 2010, 133, 014101.	1.2	227
13	Tensor hypercontraction density fitting. I. Quartic scaling second- and third-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2012, 137, 044103.	1.2	210
14	Large-scale symmetry-adapted perturbation theory computations via density fitting and Laplace transformation techniques: Investigating the fundamental forces of DNA-intercalator interactions. Journal of Chemical Physics, 2011, 135, 174107.	1.2	174
15	Tensor hypercontraction. II. Least-squares renormalization. Journal of Chemical Physics, 2012, 137, 224106.	1.2	162
16	Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver. Physical Review Letters, 2019, 122, 230401.	2.9	150
17	<scp>TeraChem</scp>: A graphical processing unit<scp>â€accelerated</scp> electronic structure package for <scp>largeâ€scale</scp> ab initio molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1494.	6.2	143
18	Communication: Tensor hypercontraction. III. Least-squares tensor hypercontraction for the determination of correlated wavefunctions. Journal of Chemical Physics, 2012, 137, 221101.	1.2	135

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19	Origin of the Surprising Enhancement of Electrostatic Energies by Electron-Donating Substituents in Substituted Sandwich Benzene Dimers. Journal of the American Chemical Society, 2011, 133, 13244-13247.	6.6	130
20	Improvement of the coupled-cluster singles and doubles method via scaling same- and opposite-spin components of the double excitation correlation energy. Journal of Chemical Physics, 2008, 128, 124111.	1.2	123
21	Accurate Prediction of Noncovalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test Set. Journal of Chemical Theory and Computation, 2012, 8, 2835-2843.	2.3	98
22	An atomic orbital-based formulation of the complete active space self-consistent field method on graphical processing units. Journal of Chemical Physics, 2015, 142, 224103.	1.2	98
23	Efficient evaluation of triple excitations in symmetry-adapted perturbation theory via second-order MÃ¸llerâ€“Plesset perturbation theory natural orbitals. Journal of Chemical Physics, 2010, 133, 104107.	1.2	95
24	Assessment of standard force field models against highâ€qualityab initiopotential curves for prototypes of Ï€âˆ’Ï€, CH/Ï€, and SH/Ï€ interactions. Journal of Computational Chemistry, 2009, 30, 2187-2193.	1.5	93
25	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. Journal of Chemical Physics, 2020, 152, 224110.	1.2	87
26	Quantum-Mechanical Analysis of the Energetic Contributions to Ï€ Stacking in Nucleic Acids versus Rise, Twist, and Slide. Journal of the American Chemical Society, 2013, 135, 1306-1316.	6.6	80
27	Determination of Hydrogen Bond Structure in Water versus Aprotic Environments To Test the Relationship Between Length and Stability. Journal of the American Chemical Society, 2015, 137, 5730-5740.	6.6	75
28	Quartic scaling second-order approximate coupled cluster singles and doubles via tensor hypercontraction: THC-CC2. Journal of Chemical Physics, 2013, 138, 124111.	1.2	66
29	Atomistic non-adiabatic dynamics of the LH2 complex with a GPU-accelerated ab initio exciton model. Physical Chemistry Chemical Physics, 2017, 19, 14924-14936.	1.3	64
30	Accurately Characterizing the Ï€âˆ’Ï€ Interaction Energies of Indoleâˆ’Benzene Complexes. Journal of Physical Chemistry A, 2010, 114, 3576-3582.	1.1	63
31	Reactive desorption electrospray ionization mass spectrometry (DESI-MS) of natural products of a marine alga. Analytical and Bioanalytical Chemistry, 2009, 394, 245-254.	1.9	61
32	Exact Tensor Hypercontraction: A Universal Technique for the Resolution of Matrix Elements of Local Finite-Range<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>-Body Potentials in Many-Body Quantum Problems. Physical Review Letters, 2013, 111, 132505.	2.9	61
33	An atomic orbital-based formulation of analytical gradients and nonadiabatic coupling vector elements for the state-averaged complete active space self-consistent field method on graphical processing units. Journal of Chemical Physics, 2015, 143, 154107.	1.2	60
34	Communication: Acceleration of coupled cluster singles and doubles via orbital-weighted least-squares tensor hypercontraction. Journal of Chemical Physics, 2014, 140, 181102.	1.2	57
35	Tensor Hypercontraction Equation-of-Motion Second-Order Approximate Coupled Cluster: Electronic Excitation Energies in O(N4) Time. Journal of Physical Chemistry B, 2013, 117, 12972-12978.	1.2	54
36	Nonadiabatic Ab Initio Molecular Dynamics with the Floating Occupation Molecular Orbital-Complete Active Space Configuration Interaction Method. Journal of Chemical Theory and Computation, 2018, 14, 339-350.	2.3	53

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37	A direct-compatible formulation of the coupled perturbed complete active space self-consistent field equations on graphical processing units. Journal of Chemical Physics, 2017, 146, 174113.	1.2	50
38	Tensor Hypercontraction Second-Order MÃ¸llerâ€“Plesset Perturbation Theory: Grid Optimization and Reaction Energies. Journal of Chemical Theory and Computation, 2015, 11, 3042-3052.	2.3	47
39	Accurate Interaction Energies for Problematic Dispersion-Bound Complexes: Homogeneous Dimers of NCCN, P2, and PCCP. Journal of Chemical Theory and Computation, 2011, 7, 2842-2851.	2.3	46
40	Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Excited to the nÏ€* and Ï€Ï€* Excited States. Journal of the American Chemical Society, 2020, 142, 20680-20690.	6.6	46
41	Discrete variable representation in electronic structure theory: Quadrature grids for least-squares tensor hypercontraction. Journal of Chemical Physics, 2013, 138, 194107.	1.2	45
42	Tractability gains in symmetry-adapted perturbation theory including coupled double excitations: CCD+ST(CCD) dispersion with natural orbital truncations. Journal of Chemical Physics, 2013, 139, 174102.	1.2	44
43	Analytic first derivatives of floating occupation molecular orbital-complete active space configuration interaction on graphical processing units. Journal of Chemical Physics, 2015, 143, 014111.	1.2	44
44	Configuration interaction singles natural orbitals: An orbital basis for an efficient and size intensive multireference description of electronic excited states. Journal of Chemical Physics, 2015, 142, 024102.	1.2	43
45	Excited-State Dynamics of 2-(2â€²-Hydroxyphenyl)benzothiazole: Ultrafast Proton Transfer and Internal Conversion. Journal of Physical Chemistry A, 2017, 121, 4595-4605.	1.1	43
46	Desorption electrospray ionization reactions between host crown ethers and the influenza neuraminidase inhibitor oseltamivir for the rapid screening of TamifluÂ®. Analyst, The, 2008, 133, 1513.	1.7	40
47	Rank reduced coupled cluster theory. I. Ground state energies and wavefunctions. Journal of Chemical Physics, 2019, 150, 164118.	1.2	37
48	Made From Henna! A Fast-Charging, High-Capacity, and Recyclable Tetrakislawsone Cathode Material for Lithium Ion Batteries. ACS Sustainable Chemistry and Engineering, 2019, 7, 13836-13844.	3.2	36
49	Analytic formulation of derivative coupling vectors for complete active space configuration interaction wavefunctions with floating occupation molecular orbitals. Journal of Chemical Physics, 2016, 145, 174110.	1.2	35
50	Holeâ€“hole Tammâ€“Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation. Journal of Chemical Physics, 2020, 153, 024110.	1.2	34
51	Ab Initio Nonadiabatic Molecular Dynamics with Holeâ€“Hole Tammâ€“Dancoff Approximated Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 5499-5511.	2.3	27
52	Improved Complete Active Space Configuration Interaction Energies with a Simple Correction from Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 1130-1146.	2.3	26
53	Complete active space configuration interaction from state-averaged configuration interaction singles natural orbitals: Analytic first derivatives and derivative coupling vectors. Journal of Chemical Physics, 2017, 147, 094104.	1.2	25
54	Mechanism for the Enhanced Excited-State Lewis Acidity of Methyl Viologen. Journal of the American Chemical Society, 2016, 138, 1868-1876.	6.6	24

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55	Nonadiabatic Dynamics of Photoexcited cis-Stilbene Using Ab Initio Multiple Spawning. Journal of Physical Chemistry B, 2020, 124, 5476-5487.	1.2	24
56	â€œBalancingâ€•the Block Davidsonâ€“Liu Algorithm. Journal of Chemical Theory and Computation, 2016, 12, 3003-3007.	2.3	23
57	Effect of Nonplanarity on Excited-State Proton Transfer and Internal Conversion in Salicylideneaniline. Journal of Physical Chemistry A, 2018, 122, 5555-5562.	1.1	23
58	Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures. Journal of Chemical Theory and Computation, 2020, 16, 4021-4028.	2.3	22
59	Rotational state analysis of AlH+ by two-photon dissociation. Journal of Molecular Spectroscopy, 2014, 300, 108-111.	0.4	20
60	Excited-State Dynamics of a Benzotriazole Photostabilizer: 2-(2â€²-Hydroxy-5â€²-methylphenyl)benzotriazole. Journal of Physical Chemistry A, 2017, 121, 6377-6387.	1.1	20
61	Robust and Efficient Spin Purification for Determinantal Configuration Interaction. Journal of Chemical Theory and Computation, 2017, 13, 4162-4172.	2.3	17
62	Rank-reduced coupled-cluster. III. Tensor hypercontraction of the doubles amplitudes. Journal of Chemical Physics, 2022, 156, 054102.	1.2	15
63	Nature-Derived Sodium-Ion Battery: Mechanistic Insights into Na-Ion Coordination within Sustainable Molecular Cathode Materials. ACS Applied Energy Materials, 2019, 2, 8596-8604.	2.5	14
64	Rank reduced coupled cluster theory. II. Equation-of-motion coupled-cluster singles and doubles. Journal of Chemical Physics, 2019, 151, 164121.	1.2	13
65	Stereoisomer specific reaction of hexabromocyclododecane with reduced sulfur species in aqueous solutions. Chemosphere, 2019, 226, 238-245.	4.2	12
66	Competition Between Ï€â€“Ï€ and Cï£¿H/Ï€ Interactions: A Comparison of the Structural and Electronic Properties of Alkoxyâ€Substituted 1,8â€Bis((propyloxyphenyl)ethynyl)naphthalenes. Chemistry - A European Journal, 2015, 21, 19168-19175.	1.7	9
67	Strong, Nonresonant Radiation Enhances Cisâ€“Trans Photoisomerization of Stilbene in Solution. Journal of Physical Chemistry A, 2020, 124, 5999-6008.	1.1	7
68	GPU acceleration of rank-reduced coupled-cluster singles and doubles. Journal of Chemical Physics, 2021, 155, 184110.	1.2	6
69	Cover Image, Volume 11, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1523.	6.2	5
70	Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Holeâ€“Hole Tammâ€“Dancoff-Approximated Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 7120-7133.	2.3	3
71	I<scp>ntera</scp>C<scp>hem</scp>: Exploring Excited States in Virtual Reality with Ab Initio Interactive Molecular Dynamics. Journal of Chemical Theory and Computation, 0, , .	2.3	3
72	Comment on â€œPositive semidefinite tensor factorizations of the two-electron integral matrix for low-scalingab initioelectronic structureâ€•[J. Chem. Phys. 143, 064103 (2015)]. Journal of Chemical Physics, 2016, 145, 027101.	1.2	1