C David Sherrill

List of Publications by Year
in descending order

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		7069	5663
202	27,374	78	162
papers	citations	h-index	g-index

210	210	210	19019
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Estimates of the Ab Initio Limit for Ï€â^Ï€ Interactions:â€‰ The Benzene Dimer. Journal of the American Chemical Society, 2002, 124, 10887-10893.	6.6	1,229
4	<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
5	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	6.2	838
6	High-Accuracy Quantum Mechanical Studies of Ï€â^Ï€ Interactions in Benzene Dimers. Journal of Physical Chemistry A, 2006, 110, 10656-10668.	1.1	711
7	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
8	Highly Accurate Coupled Cluster Potential Energy Curves for the Benzene Dimer:Â Sandwich, T-Shaped, and Parallel-Displaced Configurations. Journal of Physical Chemistry A, 2004, 108, 10200-10207.	1.1	647
9	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	1.5	617
10	Density-functional approaches to noncovalent interactions: A comparison of dispersion corrections (DFT-D), exchange-hole dipole moment (XDM) theory, and specialized functionals. Journal of Chemical Physics, 2011, 134, 084107.	1.2	607
11	Substituent Effects in Ï€â^Ï€ Interactions:Â Sandwich and T-Shaped Configurations. Journal of the American Chemical Society, 2004, 126, 7690-7697.	6.6	606
12	Levels of symmetry adapted perturbation theory (SAPT). I. Efficiency and performance for interaction energies. Journal of Chemical Physics, 2014, 140, 094106.	1.2	589
13	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
14	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
15	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
16	Wavefunction methods for noncovalent interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 304-326.	6.2	345
17	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
18	Basis set consistent revision of the S22 test set of noncovalent interaction energies. Journal of Chemical Physics, 2010, 132, 144104.	1.2	309

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19	Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory. Journal of Physical Chemistry Letters, 2016, 7, 2197-2203.	2.1	305
20	Energy Component Analysis of Ï€ Interactions. Accounts of Chemical Research, 2013, 46, 1020-1028.	7.6	297
21	Basis set convergence of the coupled-cluster correction, $delta _{ext{MP2}}^{ext{CCSD(T)}}$Î MP2CCSD(T): Best practices for benchmarking non-covalent interactions and the attendant revision of the S22, NBC10, HBC6, and HSG databases. Journal of Chemical Physics, 2011, 135, 194102.	1.2	295
22	The Configuration Interaction Method: Advances in Highly Correlated Approaches. Advances in Quantum Chemistry, 1999, , 143-269.	0.4	294
23	Unexpected Substituent Effects in Face-to-Face Ï€-Stacking Interactions. Journal of Physical Chemistry A, 2003, 107, 8377-8379.	1.1	276
24	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
25	PSI3: An open-source Ab Initio electronic structure package. Journal of Computational Chemistry, 2007, 28, 1610-1616.	1.5	258
26	Energies and analytic gradients for a coupled-cluster doubles model using variational Brueckner orbitals: Application to symmetry breaking in O4+. Journal of Chemical Physics, 1998, 109, 4171-4181.	1.2	228
27	Density fitting of intramonomer correlation effects in symmetry-adapted perturbation theory. Journal of Chemical Physics, 2010, 133, 014101.	1.2	227
28	Size-consistent wave functions for nondynamical correlation energy: The valence active space optimized orbital coupled-cluster doubles model. Journal of Chemical Physics, 1998, 109, 10669-10678.	1.2	222
29	The Effect of Multiple Substituents on Sandwich and T-Shaped Ï€â€“Ï€ Interactions. Chemistry - A European Journal, 2006, 12, 3821-3828.	1.7	197
30	Perturbative corrections to the equation-of-motion spinâ€“flip self-consistent field model: Application to bond-breaking and equilibrium properties of diradicals. Journal of Chemical Physics, 2002, 116, 3194-3203.	1.2	192
31	Aliphatic Câˆ’H/Ï€ Interactions:Â Methaneâˆ’Benzene, Methaneâˆ’Phenol, and Methaneâˆ’Indole Complexes. Journal of Physical Chemistry A, 2006, 110, 10822-10828.	1.1	177
32	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
33	Comparing Counterpoise-Corrected, Uncorrected, and Averaged Binding Energies for Benchmarking Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 49-57.	2.3	166
34	Models of S/Ï€ interactions in protein structures: Comparison of the H₂Sâ€“benzene complex with PDB data. Protein Science, 2007, 16, 2216-2223.	3.1	164
35	Tensor hypercontraction. II. Least-squares renormalization. Journal of Chemical Physics, 2012, 137, 224106.	1.2	162
36	Second-order perturbation corrections to singles and doubles coupled-cluster methods: General theory and application to the valence optimized doubles model. Journal of Chemical Physics, 2000, 113, 3548-3560.	1.2	155

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37	Beyond the Benzene Dimer:â€‰ An Investigation of the Additivity of Ï€âˆ’Ï€ Interactions. Journal of Physical Chemistry A, 2005, 109, 10475-10478.	1.1	155
38	Oscillations in meta-generalized-gradient approximation potential energy surfaces for dispersion-bound complexes. Journal of Chemical Physics, 2009, 131, 034111.	1.2	153
39	Substituent effects in parallel-displaced Ï€â€“Ï€ interactions. Physical Chemistry Chemical Physics, 2008, 10, 2646.	1.3	149
40	Investigations into the Stability of Tethered Palladium(II) Pincer Complexes during Heck Catalysis. Organometallics, 2005, 24, 4351-4361.	1.1	147
41	Frontiers in electronic structure theory. Journal of Chemical Physics, 2010, 132, 110902.	1.2	147
42	The Theoretical Prediction of Molecular Radical Species:â€‰ a Systematic Study of Equilibrium Geometries and Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2001, 105, 9736-9747.	1.1	142
43	A spin-complete version of the spin-flip approach to bond breaking: What is the impact of obtaining spin eigenfunctions?. Journal of Chemical Physics, 2003, 118, 9084-9094.	1.2	142
44	Potential Energy Curves for Cationâˆ’Ï€ Interactions: Off-Axis Configurations Are Also Attractive. Journal of Physical Chemistry A, 2009, 113, 13628-13632.	1.1	135
45	Communication: Tensor hypercontraction. III. Least-squares tensor hypercontraction for the determination of correlated wavefunctions. Journal of Chemical Physics, 2012, 137, 221101.	1.2	135
46	Substituent Effects in Sandwich Configurations of Multiply Substituted Benzene Dimers Are Not Solely Governed By Electrostatic Control. Journal of the American Chemical Society, 2009, 131, 4574-4575.	6.6	132
47	Accuracy and Efficiency of Coupled-Cluster Theory Using Density Fitting/Cholesky Decomposition, Frozen Natural Orbitals, and a t₁-Transformed Hamiltonian. Journal of Chemical Theory and Computation, 2013, 9, 2687-2696.	2.3	131
48	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
49	Full configuration interaction potential energy curves for the Xâ€Š1Î£g+, Bâ€Š1Î”g, and Bâ€²â€Š1Î£g+ states of C2: A challenge for approximate methods. Journal of Chemical Physics, 2004, 121, 9211-9219.	1.2	127
50	Formal Estimation of Errors in Computed Absolute Interaction Energies of Proteinâˆ’Ligand Complexes. Journal of Chemical Theory and Computation, 2011, 7, 790-797.	2.3	127
51	Is Mo/llerâ€“Plesset perturbation theory a convergent ab initio method?. Journal of Chemical Physics, 2000, 112, 9213-9222.	1.2	125
52	Excited states theory for optimized orbitals and valence optimized orbitals coupled-cluster doubles models. Journal of Chemical Physics, 2000, 113, 6509-6527.	1.2	125
53	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
54	The diagonal Bornâ€“Oppenheimer correction beyond the Hartreeâ€“Fock approximation. Journal of Chemical Physics, 2003, 118, 3921-3927.	1.2	122

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55	Full configuration interaction potential energy curves for breaking bonds to hydrogen: An assessment of single-reference correlation methods. Journal of Chemical Physics, 2003, 118, 1610-1619.	1.2	115
56	Estimates of the ab Initio Limit for Sulfurâ^Ï€ Interactions:â€‰ The H2Sâ^'Benzene Dimer. Journal of Physical Chemistry A, 2005, 109, 191-196.	1.1	108
57	Performance of spin-component-scaled MÃ¸llerâ€“Plesset theory (SCS-MP2) for potential energy curves of noncovalent interactions. Physical Chemistry Chemical Physics, 2007, 9, 6106.	1.3	108
58	Quantum-Mechanical Evaluation of Ï€â€“Ï€ versus Substituentâ^Ï€ Interactions in Ï€ Stacking: Direct Evidence for the Wheelerâ€“Houk Picture. Journal of the American Chemical Society, 2014, 136, 17386-17389.	6.6	107
59	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	2.3	106
60	Quadratically convergent algorithm for orbital optimization in the orbital-optimized coupled-cluster doubles method and in orbital-optimized second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2011, 135, 104103.	1.2	104
61	Chemical Assignment of Symmetry-Adapted Perturbation Theory Interaction Energy Components: The Functional-Group SAPT Partition. Journal of Chemical Theory and Computation, 2014, 10, 4417-4431.	2.3	101
62	The XÎ£g+1, BÎ”g1, and Bâ€²Î£g+1 states of C2: A comparison of renormalized coupled-cluster and multireference methods with full configuration interaction benchmarks. Journal of Chemical Physics, 2005, 122, 124104.	1.2	99
63	Redox-Active Ligands Facilitate Bimetallic O₂Homolysis at Five-Coordinate Oxorhenium(V) Centers. Journal of the American Chemical Society, 2010, 132, 3879-3892.	6.6	98
64	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
65	N8: A Structure Analogous to Pentalene, and Other High-Energy Density Minima. The Journal of Physical Chemistry, 1995, 99, 2324-2328.	2.9	97
66	First Principles Computation of Lattice Energies of Organic Solids: The Benzene Crystal. Chemistry - A European Journal, 2008, 14, 2542-2547.	1.7	95
67	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
68	Structures and vibrational frequencies in the full configuration interaction limit: Predictions for four electronic states of methylene using a triple-zeta plus double polarization (TZ2P) basis. Journal of Chemical Physics, 1998, 108, 1040-1049.	1.2	93
69	Assessment of standard force field models against highâ€qualityab initiopotential curves for prototypes of Ï€â€“Ï€, CH/Ï€, and SH/Ï€ interactions. Journal of Computational Chemistry, 2009, 30, 2187-2193.	1.5	93
70	An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations. Journal of Chemical Theory and Computation, 2010, 6, 727-734.	2.3	91
71	ISOTOPIC RATIOS IN TITAN's METHANE: MEASUREMENTS AND MODELING. Astrophysical Journal, 2012, 749, 159.	1.6	91
72	Benchmark full configuration interaction and equation-of-motion coupled-cluster model with single and double substitutions for ionized systems results for prototypical charge transfer systems: Noncovalent ionized dimers. Journal of Chemical Physics, 2007, 127, 164110.	1.2	85

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73	The electron and nuclear orbitals model: current challenges and future prospects. Molecular Physics, 2004, 102, 111-123.	0.8	84
74	On the relationship between bond-length alternation and many-electron self-interaction error. Journal of Chemical Physics, 2012, 137, 124305.	1.2	84
75	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. Journal of Chemical Physics, 2017, 147, 161727.	1.2	82
76	Appointing silver and bronze standards for noncovalent interactions: A comparison of spin-component-scaled (SCS), explicitly correlated (F12), and specialized wavefunction approaches. Journal of Chemical Physics, 2014, 141, 234111.	1.2	81
77	Do Deuteriums Form Stronger CHâ^'Ï€ Interactions?. Journal of the American Chemical Society, 2012, 134, 14306-14309.	6.6	80
78	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
79	Spatial assignment of symmetry adapted perturbation theory interaction energy components: The atomic SAPT partition. Journal of Chemical Physics, 2014, 141, 044115.	1.2	76
80	On the accuracy limits of orbital expansion methods: Explicit effects ofk-functions on atomic and molecular energies. Journal of Chemical Physics, 2003, 118, 8594-8610.	1.2	70
81	Challenges of laser-cooling molecular ions. New Journal of Physics, 2011, 13, 063023.	1.2	70
82	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules I. Reference Data at the CCSD(T) Complete Basis Set Limit. Journal of Chemical Theory and Computation, 2016, 12, 595-604.	2.3	69
83	Communication: Resolving the three-body contribution to the lattice energy of crystalline benzene: Benchmark results from coupled-cluster theory. Journal of Chemical Physics, 2014, 140, 121104.	1.2	68
84	Intramolecular Noncovalent Interactions Facilitate Thermally Activated Delayed Fluorescence (TADF). Journal of Physical Chemistry Letters, 2019, 10, 3260-3268.	2.1	68
85	Natural orbitals as substitutes for optimized orbitals in complete active space wavefunctions. Chemical Physics Letters, 2004, 395, 227-232.	1.2	67
86	TheXÌƒ3B1,Ã£1A1,bÌƒ1B1, andcÌƒ1A1Electronic States of CH2. The Journal of Physical Chemistry, 1996, 100, 7911-7918.	2.9	65
87	Closs's diradical: some surprises on the potential energy hypersurface. The Journal of Physical Chemistry, 1992, 96, 3712-3716.	2.9	63
88	Accurately Characterizing the Ï€â^'Ï€ Interaction Energies of Indoleâ^'Benzene Complexes. Journal of Physical Chemistry A, 2010, 114, 3576-3582.	1.1	63
89	Accurate Noncovalent Interaction Energies Using Truncated Basis Sets Based on Frozen Natural Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 293-299.	2.3	62
90	Communication: Practical intramolecular symmetry adapted perturbation theory via Hartree-Fock embedding. Journal of Chemical Physics, 2015, 143, 051103.	1.2	62

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91	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
92	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
93	Assessment of the performance of tuned range-separated hybrid density functionals in predicting accurate quasiparticle spectra. Physical Review B, 2012, 86, .	1.1	58
94	Buckyplates and Buckybowls: Examining the Effects of Curvature on Ï€â€“Ï€ Interactions. Journal of Physical Chemistry A, 2012, 116, 11920-11926.	1.1	58
95	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
96	Rubrene: The Interplay between Intramolecular and Intermolecular Interactions Determines the Planarization of Its Tetracene Core in the Solid State. Journal of the American Chemical Society, 2015, 137, 8775-8782.	6.6	56
97	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron-Propagator Methods. Journal of Chemical Theory and Computation, 2016, 12, 627-637.	2.3	56
98	Assessment of Empirical Models versus High-Accuracy Ab Initio Methods for Nucleobase Stacking: Evaluating the Importance of Charge Penetration. Journal of Chemical Theory and Computation, 2015, 11, 4197-4204.	2.3	51
99	High-Level ab Initio Studies of Hydrogen Abstraction from Prototype Hydrocarbon Systems. Journal of Physical Chemistry A, 2006, 110, 11160-11173.	1.1	49
100	Orbital-optimized coupled-electron pair theory and its analytic gradients: Accurate equilibrium geometries, harmonic vibrational frequencies, and hydrogen transfer reactions. Journal of Chemical Physics, 2013, 139, 054104.	1.2	48
101	Analytic energy gradients for the orbital-optimized second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 184103.	1.2	48
102	Density-fitted singles and doubles coupled cluster on graphics processing units. Molecular Physics, 2014, 112, 844-852.	0.8	48
103	Comparison of Explicitly Correlated Methods for Computing High-Accuracy Benchmark Energies for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2017, 13, 86-99.	2.3	48
104	The Energy Computation Paradox and ab initio Protein Folding. PLoS ONE, 2011, 6, e18868.	1.1	48
105	Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices. Journal of Computational Chemistry, 2001, 22, 1574-1589.	1.5	46
106	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
107	Discrete variable representation in electronic structure theory: Quadrature grids for least-squares tensor hypercontraction. Journal of Chemical Physics, 2013, 138, 194107.	1.2	45
108	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

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109	Compact Variational Wave Functions Incorporating Limited Triple and Quadruple Substitutions. The Journal of Physical Chemistry, 1996, 100, 6069-6075.	2.9	43
110	The electronic structure of oxo-Mn(salen): Single-reference and multireference approaches. Journal of Chemical Physics, 2006, 124, 144314.	1.2	43
111	A Versatile Co(bisalen) Unit for Homogeneous and Heterogeneous Cooperative Catalysis in the Hydrolytic Kinetic Resolution of Epoxides. Chemistry - A European Journal, 2009, 15, 3951-3955.	1.7	42
112	AP-Net: An atomic-pairwise neural network for smooth and transferable interaction potentials. Journal of Chemical Physics, 2020, 153, 044112.	1.2	41
113	Benchmark configuration interaction spectroscopic constants for Xâ€‰1Î£g+â€‰C2 and Xâ€‰1Î£+â€‰CN+. Journal of Chemical Physics, 1998, 108, 6717-6721.	1.2	40
114	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
115	Density-fitted open-shell symmetry-adapted perturbation theory and application to Ï€-stacking in benzene dimer cation and ionized DNA base pair steps. Journal of Chemical Physics, 2016, 145, 134106.	1.2	40
116	The performance of density functional theory for equilibrium molecular properties of symmetry breaking molecules. Journal of Chemical Physics, 2001, 114, 8257-8269.	1.2	39
117	Density functional theory predictions of anharmonicity and spectroscopic constants for diatomic molecules. Journal of Chemical Physics, 2001, 115, 2439-2448.	1.2	39
118	A comparison of polarized double-zeta basis sets and natural orbitals for full configuration interaction benchmarks. Journal of Chemical Physics, 2003, 118, 1604-1609.	1.2	39
119	Dispersion-Weighted Explicitly Correlated Coupled-Cluster Theory [DW-CCSD(T**)-F12]. Journal of Chemical Theory and Computation, 2011, 7, 3978-3982.	2.3	38
120	An Assessment of the Accuracy of Multireference Configuration Interaction (MRCI) and Complete-Active-Space Second-Order Perturbation Theory (CASPT2) for Breaking Bonds to Hydrogen. Journal of Physical Chemistry A, 2003, 107, 5611-5616.	1.1	36
121	Important configurations in configuration interaction and coupled-cluster wave functions. Chemical Physics Letters, 2005, 412, 121-124.	1.2	36
122	High accuracy ab initio studies of Li6+, Li6â^', and three isomers of Li6. Journal of Chemical Physics, 2005, 122, 064315.	1.2	36
123	Assessing the Performance of Density Functional Theory for the Electronic Structure of Metalâ^'Salens:â€‰ The 3d⁰-Metals. Journal of Physical Chemistry A, 2008, 112, 3466-3477.	1.1	36
124	The bigger, the better: Ring-size effects of macrocyclic oligomeric Co(iii)-salen catalysts. Chemical Science, 2011, 2, 429-438.	3.7	36
125	Assessing the Performance of Density Functional Theory for the Electronic Structure of Metalâ^'Salens: The M06 Suite of Functionals and the d⁴-Metals. Journal of Physical Chemistry A, 2010, 114, 11714-11718.	1.1	35
126	Analytic energy gradients for the coupled-cluster singles and doubles with perturbative triples method with the density-fitting approximation. Journal of Chemical Physics, 2017, 147, 044104.	1.2	34

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127	Electronic structure software. Journal of Chemical Physics, 2020, 153, 070401.	1.2	34
128	XÌƒ 3B1, Ã£ 1A1, bÌƒ 1B1, and cÌƒ 1 Electronic States of. Journal of Physical Chemistry A, 1998, 102, 3999-4006.	1.1	33
129	Assessing the Performance of Density Functional Theory for the Electronic Structure of Metalâ^'Salens: The d²-Metals. Journal of Physical Chemistry A, 2008, 112, 6741-6752.	1.1	33
130	A Comparison of One-Particle Basis Set Completeness, Higher-Order Electron Correlation, Relativistic Effects, and Adiabatic Corrections for Spectroscopic Constants of BH, CH+, and NHâ€. Journal of Physical Chemistry A, 2004, 108, 3068-3075.	1.1	32
131	Orbital-optimized MP2.5 and its analytic gradients: Approaching CCSD(T) quality for noncovalent interactions. Journal of Chemical Physics, 2014, 141, 204105.	1.2	32
132	Accurate description of torsion potentials in conjugated polymers using density functionals with reduced self-interaction error. Journal of Chemical Physics, 2014, 140, 054310.	1.2	32
133	Analytic energy gradients for the coupled-cluster singles and doubles method with the density-fitting approximation. Journal of Chemical Physics, 2016, 144, 174103.	1.2	32
134	Understanding the Many-Body Basis Set Superposition Error: Beyond Boys and Bernardi. Journal of Chemical Theory and Computation, 2018, 14, 2386-2400.	2.3	32
135	Tipping the Balance between S-Ï€ and O-Ï€ Interactions. Journal of the American Chemical Society, 2018, 140, 13301-13307.	6.6	32
136	The XËœ 1 A 1 , aËœ 3 B 1 , aËœ 1 BËœ 1 , and BËœ 1 A 1 electronic states of SiH 2. Theoretical Chemistry Accounts, 1997, 97, 341-349.	0.5	31
137	Assessing the Performance of Density Functional Theory for the Electronic Structure of Metalâ^'Salens: The d⁶-Metals. Journal of Physical Chemistry A, 2009, 113, 9231-9236.	1.1	30
138	Macrocyclic Cyclooctaneâ€Supported AlClâ€“Salen Catalysts for Conjugated Addition Reactions: Effect of Linker and Support Structure on Catalysis. Chemistry - A European Journal, 2009, 15, 1186-1194.	1.7	29
139	A Tyrosine-Rich Cell Surface Protein in the Diatom Amphora coffeaeformis Identified through Transcriptome Analysis and Genetic Transformation. PLoS ONE, 2014, 9, e110369.	1.1	29
140	Acetylene: Synergy between theory and experiment. Journal of Chemical Physics, 1993, 98, 8384-8391.	1.2	28
141	1-Silavinylidene: The First Unsaturated Silylene. The Journal of Physical Chemistry, 1995, 99, 1949-1952.	2.9	28
142	The AÌƒâ€‰1Au state and the T2 potential surface of acetylene: Implications for triplet perturbations in the fluorescence spectra of the AÌƒ state. Journal of Chemical Physics, 1996, 104, 8507-8515.	1.2	28
143	X-ray Structures, Photophysical Characterization, and Computational Analysis of Geometrically Constrained Copper(I)â^'Phenanthroline Complexes. Inorganic Chemistry, 2003, 42, 4918-4929.	1.9	28
144	The Surprising Importance of Peptide Bond Contacts in Drugâ€“Protein Interactions. Chemistry - A European Journal, 2017, 23, 7887-7890.	1.7	28

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145	Assessment of Density Functional Methods for Geometry Optimization of Bimolecular van der Waals Complexes. Journal of Chemical Theory and Computation, 2018, 14, 3004-3013.	2.3	27
146	Approaches for machine learning intermolecular interaction energies and application to energy components from symmetry adapted perturbation theory. Journal of Chemical Physics, 2020, 152, 074103.	1.2	25
147	Complete basis set extrapolations for low-lying triplet electronic states of acetylene and vinylidene. Journal of Chemical Physics, 2000, 113, 1447-1454.	1.2	24
148	XÌƒÂ1A1, Ã£Â3B1, ÃƒÂ1B1, and BÌƒÂ1A1Electronic States of. Journal of Physical Chemistry A, 1997, 101, 6955-6963.	1.1	23
149	Analysis of transition state stabilization by non-covalent interactions in the Houkâ€“List model of organocatalyzed intermolecular Aldol additions using functional-group symmetry-adapted perturbation theory. Physical Chemistry Chemical Physics, 2016, 18, 10297-10308.	1.3	23
150	The AÌƒ 1Aâ€˜ state of isocyanogen (CNCN). Journal of Chemical Physics, 1994, 100, 8920-8924.	1.2	22
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