David P Tew

List of Publications by Year
in descending order

116	18,573	87723	22102
papers	citations	38 h-index	113 g-index

117	117	117	16950
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A new hybrid exchangeâ€“correlation functional using the Coulomb-attenuating method (CAM-B3LYP). Chemical Physics Letters, 2004, 393, 51-57.	1.2	11,492
2	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
3	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
4	Explicitly Correlated Electrons in Molecules. Chemical Reviews, 2012, 112, 4-74.	23.0	487
5	Communications: Accurate and efficient approximations to explicitly correlated coupled-cluster singles and doubles, CCSD-F12. Journal of Chemical Physics, 2010, 132, 231102.	1.2	259
6	Quintuple-Î¶ quality coupled-cluster correlation energies with triple-Î¶ basis sets. Physical Chemistry Chemical Physics, 2007, 9, 1921-1930.	1.3	244
7	Basis-set extrapolation techniques for the accurate calculation of molecular equilibrium geometries using coupled-cluster theory. Journal of Chemical Physics, 2006, 125, 044108.	1.2	233
8	New correlation factors for explicitly correlated electronic wave functions. Journal of Chemical Physics, 2005, 123, 074101.	1.2	231
9	Quantitative quantum chemistry. Molecular Physics, 2008, 106, 2107-2143.	0.8	215
10	Simulating the vibrational quantum dynamics of molecules using photonics. Nature, 2018, 557, 660-667.	13.7	159
11	Full-dimensional quantum calculations of ground-state tunneling splitting of malonaldehyde using an accurate ab initio potential energy surface. Journal of Chemical Physics, 2008, 128, 224314.	1.2	149
12	Witnessing eigenstates for quantum simulation of Hamiltonian spectra. Science Advances, 2018, 4, eaap9646.	4.7	142
13	Experimental Bayesian Quantum Phase Estimation on a Silicon Photonic Chip. Physical Review Letters, 2017, 118, 100503.	2.9	123
14	A diagonal orbital-invariant explicitly-correlated coupled-cluster method. Chemical Physics Letters, 2008, 452, 326-332.	1.2	118
15	Criegee Intermediate Reactions with Carboxylic Acids: A Potential Source of Secondary Organic Aerosol in the Atmosphere. ACS Earth and Space Chemistry, 2018, 2, 833-842.	1.2	102
16	The MP2â€F12 method in the T<scp>URBOMOLE</scp> program package. Journal of Computational Chemistry, 2011, 32, 2492-2513.	1.5	98
17	Basis Set Limit CCSD(T) Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2007, 111, 11242-11248.	1.1	92
18	Atomization energies from coupled-cluster calculations augmented with explicitly-correlated perturbation theory. Chemical Physics, 2009, 356, 14-24.	0.9	92

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19	Explicitly correlated PNO-MP2 and PNO-CCSD and their application to the S66 set and large molecular systems. Physical Chemistry Chemical Physics, 2014, 16, 22167-22178.	1.3	92
20	Local explicitly correlated second-order MÃ¸llerâ€“Plesset perturbation theory with pair natural orbitals. Journal of Chemical Physics, 2011, 135, 074107.	1.2	87
21	Implementation of the full explicitly correlated coupled-cluster singles and doubles model CCSD-F12 with optimally reduced auxiliary basis dependence. Journal of Chemical Physics, 2008, 129, 201103.	1.2	86
22	Local explicitly correlated second- and third-order MÃ¸llerâ€“Plesset perturbation theory with pair natural orbitals. Journal of Chemical Physics, 2012, 136, 204105.	1.2	85
23	Electron correlation: The many-body problem at the heart of chemistry. Journal of Computational Chemistry, 2007, 28, 1307-1320.	1.5	82
24	Assessment of basis sets for F12 explicitly-correlated molecular electronic-structure methods. Molecular Physics, 2009, 107, 963-975.	0.8	76
25	A comparison of linear and nonlinear correlation factors for basis set limit MÃ¸ller-Plesset second order binding energies and structures of He2, Be2, and Ne2. Journal of Chemical Physics, 2006, 125, 094302.	1.2	72
26	Accurate computational thermochemistry from explicitly correlated coupled-cluster theory. Theoretical Chemistry Accounts, 2010, 126, 289-304.	0.5	64
27	Explicitly correlated plane waves: Accelerating convergence in periodic wavefunction expansions. Journal of Chemical Physics, 2013, 139, 084112.	1.2	62
28	A reaction surface Hamiltonian study of malonaldehyde. Journal of Chemical Physics, 2006, 125, 084313.	1.2	61
29	The internal coordinate path Hamiltonian; application to methanol and malonaldehyde. Molecular Physics, 2003, 101, 3513-3525.	0.8	51
30	Role of Valence and Semicore Electron Correlation on Spin Gaps in Fe(II)-Porphyrins. Journal of Chemical Theory and Computation, 2019, 15, 1492-1497.	2.3	51
31	Efficient and accurate evaluation of potential energy matrix elements for quantum dynamics using Gaussian process regression. Journal of Chemical Physics, 2016, 145, 174112.	1.2	50
32	An explicitly correlated approach to basis set incompleteness in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2012, 137, 164112.	1.2	49
33	Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. Journal of Chemical Physics, 2018, 149, 154109.	1.2	48
34	Ab initio instanton rate theory made efficient using Gaussian process regression. Faraday Discussions, 2018, 212, 237-258.	1.6	48
35	Second order coalescence conditions of molecular wave functions. Journal of Chemical Physics, 2008, 129, 014104.	1.2	46
36	Experimental and computational studies of Criegee intermediate reactions with NH₃ and CH₃NH₂. Physical Chemistry Chemical Physics, 2019, 21, 14042-14052.	1.3	46

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37	Pair natural orbitals in explicitly correlated secondâ€order mÃ¸llerâ€“plesset theory. International Journal of Quantum Chemistry, 2013, 113, 224-229.	1.0	40
38	Similarity transformation of the electronic SchrÃ¶dinger equation via Jastrow factorization. Journal of Chemical Physics, 2019, 151, 061101.	1.2	40
39	Explicitly Correlated Coupled-Cluster Theory. Challenges and Advances in Computational Chemistry and Physics, 2010, , 535-572.	0.6	40
40	Open-shell explicitly correlated F12 methods. Molecular Physics, 2010, 108, 315-325.	0.8	39
41	Explicitly correlated coupled-cluster theory using cusp conditions. I. Perturbation analysis of coupled-cluster singles and doubles (CCSD-F12). Journal of Chemical Physics, 2010, 133, 174117.	1.2	38
42	Automated incremental scheme for explicitly correlated methods. Journal of Chemical Physics, 2010, 132, 164114.	1.2	37
43	Controlling Electronic Product Branching at Conical Intersections in the UV Photolysis of para-Substituted Thiophenols. Journal of Physical Chemistry A, 2012, 116, 12444-12459.	1.1	37
44	Understanding the reactivity bottleneck in the spin-forbidden reaction FeO++H2â†'Fe++H2O. International Journal of Mass Spectrometry, 2013, 354-355, 263-270.	0.7	37
45	Sub-meV accuracy in first-principles computations of the ionization potentials and electron affinities of the atoms H to Ne. Physical Review A, 2010, 81, .	1.0	35
46	Monohydrates of cuprous chloride and argentous chloride: H2Oâ‹…â‹…â‹…CuCl and H2Oâ‹…â‹…â‹…AgCl characterized by rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2011, 134, 134305.	1.2	35
47	The vibrations and tunnelling of malonaldehyde on a MÃ¸llerâ€“Plesset surface. Molecular Physics, 2004, 102, 2217-2226.	0.8	34
48	Characterisation of H2Sâ‹¯CuCl and H2Sâ‹¯AgCl isolated in the gas phase: A rigidly pyramidal geometry at sulphur revealed by rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2011, 135, 014307.	1.2	33
49	Molecular geometry of OCâ‹…â‹…â‹…AgI determined by broadband rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2012, 136, 064306.	1.2	30
50	Changes in the Geometries of C₂H₂ and C₂H₄ on Coordination to CuCl Revealed by Broadband Rotational Spectroscopy and ab-Initio Calculations. Inorganic Chemistry, 2014, 53, 10722-10730.	1.9	30
51	Ab Initio Vibrational Spectroscopy of cis- and trans-Formic Acid from a Global Potential Energy Surface. Journal of Physical Chemistry A, 2016, 120, 9815-9828.	1.1	30
52	Towards the Hartreeâ€“Fock and coupled-cluster singles and doubles basis set limit: A study of various models that employ single excitations into a complementary auxiliary basis set. Journal of Chemical Physics, 2010, 132, 024101.	1.2	29
53	H3Nâ‹¯Agâ€“Cl: Synthesis in a supersonic jet and characterisation by rotational spectroscopy. Chemical Physics Letters, 2010, 499, 16-20.	1.2	27
54	Distortion of ethyne on formation of a Ï€ complex with silver chloride: C2H2â‹¯Agâ€“Cl characterised by rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2012, 137, 174302.	1.2	27

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55	A second-order multi-reference perturbation method for molecular vibrations. Journal of Chemical Physics, 2013, 139, 194108.	1.2	27
56	A compact and accurate semi-global potential energy surface for malonaldehyde from constrained least squares regression. Journal of Chemical Physics, 2014, 141, 144310.	1.2	27
57	The geminal basis in explicitly correlated wave functions. Chemical Physics, 2009, 356, 25-30.	0.9	24
58	Comment on Quintuple-Î¶ quality coupled-cluster correlation energies with triple-Î¶ basis sets by D. P. Tew, W. Klopper, C. Neiss and C. HÃttig, Phys. Chem. Chem. Phys., 2007, 9, 1921 [erratum]. Physical Chemistry Chemical Physics, 2008, 10, 6325.	1.3	23
59	A prototype transition-metal olefin complex C2H4â‹¯AgCl synthesised by laser ablation and characterised by rotational spectroscopy and ab initio methods. Journal of Chemical Physics, 2011, 135, 024315.	1.2	23
60	Glyoxal studied with â€˜Multimodeâ€™, explicit large amplitude motion and anharmonicity. Physical Chemistry Chemical Physics, 2001, 3, 1958-1964.	1.3	21
61	The halogen bond between ethene and a simple perfluoroiodoalkane: C2H4â‹¯ICF3 identified by broadband rotational spectroscopy. Journal of Molecular Spectroscopy, 2012, 280, 47-53.	0.4	20
62	A GPU-accelerated immersive audio-visual framework for interaction with molecular dynamics using consumer depth sensors. Faraday Discussions, 2014, 169, 63-87.	1.6	20
63	Explicitly correlated coupled-cluster theory with Brueckner orbitals. Journal of Chemical Physics, 2016, 145, 074103.	1.2	20
64	Heat of formation of the HOSO2 radical from accurate quantum chemical calculations. Journal of Chemical Physics, 2008, 129, 114308.	1.2	19
65	Monohydrate of argentous fluoride: H2Oâ‹¯AgF characterised by rotational spectroscopy and ab initio calculations. Journal of Molecular Spectroscopy, 2011, 267, 163-168.	0.4	19
66	H2Sâ‹¯Agâ€“I synthesized by a laser-ablation method and identified by its rotational spectrum. Chemical Physics Letters, 2012, 531, 1-5.	1.2	19
67	Distortions of ethyne when complexed with a cuprous or argentous halide: the rotational spectrum of C₂H₂â‹¯CuF. Physical Chemistry Chemical Physics, 2015, 17, 19230-19237.	1.3	19
68	Non-IPR C60 solids. Journal of Chemical Physics, 2009, 130, 164705.	1.2	18
69	Geometry of an Isolated Dimer of Imidazole Characterised by Rotational Spectroscopy and Ab Initio Calculations. ChemPhysChem, 2016, 17, 1154-1158.	1.0	18
70	The Dynamics of the Reaction of FeO⁺ and H₂: A Model for Inorganic Oxidation. Angewandte Chemie - International Edition, 2017, 56, 5790-5794.	7.2	18
71	The weak orthogonality functional in explicitly correlated pair theories. Journal of Chemical Physics, 2007, 127, 174105.	1.2	17
72	The vibrations of glyoxal, studied by â€˜Multimodeâ€™, with a large amplitude motion, using an ab initio potential surface. Molecular Physics, 2001, 99, 393-402.	0.8	16

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73	Anharmonic frequencies and Berry pseudorotation motion in PF5. Chemical Physics Letters, 2003, 369, 335-344.	1.2	16
74	The Dynamics of the Reaction of FeO⁺ and H₂: A Model for Inorganic Oxidation. Angewandte Chemie, 2017, 129, 5884-5888.	1.6	16
75	A monomeric complex of ammonia and cuprous chloride: H3Nâ‹¯CuCl isolated and characterised by rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2015, 142, 144302.	1.2	15
76	A Structurally Characterized Fluoroalkyne. Angewandte Chemie - International Edition, 2017, 56, 7551-7556.	7.2	15
77	Interplay between Electronic Correlation and Metalâ€“Ligand Delocalization in the Spectroscopy of Transition Metal Compounds: Case Study on a Series of Planar Cu²⁺ Complexes. Journal of Chemical Theory and Computation, 2018, 14, 6240-6252.	2.3	15
78	Efficient and accurate description of adsorption in zeolites. Journal of Chemical Physics, 2019, 151, 234108.	1.2	15
79	Basis set extrapolation in pair natural orbital theories. Journal of Chemical Physics, 2020, 153, 174112.	1.2	15
80	An Isolated Complex of Ethyne and Gold Iodide Characterized by Broadband Rotational Spectroscopy and Ab initio Calculations. Journal of Physical Chemistry A, 2015, 119, 9636-9643.	1.1	14
81	Gas phase complexes of H₃Nâ‹¯CuF and H₃Nâ‹¯CuI studied by rotational spectroscopy and ab initio calculations: the effect of X (X = F, Cl, Br, I) in OCâ‹¯CuX and H₃Nâ‹¯CuX. Physical Chemistry Chemical Physics, 2016, 18, 13638-13645.	1.3	14
82	First UHF Implementation of the Incremental Scheme for Open-Shell Systems. Journal of Chemical Theory and Computation, 2016, 12, 65-78.	2.3	14
83	Communication: Quasi-robust local density fitting. Journal of Chemical Physics, 2018, 148, 011102.	1.2	14
84	Low energy hydrogenation products of extended Ï€ systems CnH2x: A density functional theory search strategy, benchmarked against CCSD(T), and applied to C60. Journal of Chemical Physics, 2008, 129, 114303.	1.2	13
85	H₃Pâ‹¯AgI: generation by laser-ablation and characterization by rotational spectroscopy and ab initio calculations. Physical Chemistry Chemical Physics, 2016, 18, 18971-18977.	1.3	13
86	Geometries of H2Sâ‹¯MI (M = Cu, Ag, Au) complexes studied by rotational spectroscopy: The effect of the metal atom. Journal of Chemical Physics, 2016, 145, 194306.	1.2	12
87	Molecular geometries and other properties of H2Oâ‹¯AgI and H3Nâ‹¯AgI as characterised by rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2017, 147, 234308.	1.2	12
88	Orbital-Optimized Distinguishable Cluster Theory with Explicit Correlation. Journal of Chemical Theory and Computation, 2019, 15, 13-17.	2.3	12
89	Distortion of ethyne on coordination to silver acetylide, C2H2â‹…â‹…â‹…â‹…â‹…AgCCH, characterised by broadband rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2014, 140, 124310.	1.2	11
90	Principal Domains in Local Correlation Theory. Journal of Chemical Theory and Computation, 2019, 15, 6597-6606.	2.3	11

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91	Ab initio calculation of rovibrational states for non-degenerate double-well potentials: cisâ€“trans isomerization of HOPO. Journal of Chemical Physics, 2020, 152, 174306.	1.2	11
92	Accurate Coupled Cluster Calculations of the Reaction Barrier Heights of Two CH₃^{â€¢} + CH₄ Reactions. Journal of Physical Chemistry A, 2009, 113, 11679-11684.	1.1	10
93	Molecular excited state calculations with adaptive wavefunctions on a quantum eigensolver emulation: reducing circuit depth and separating spin states. Physical Chemistry Chemical Physics, 2021, 23, 26438-26450.	1.3	10
94	Intramolecular competition between n-pair and Ï€-pair hydrogen bonding: Microwave spectrum and internal dynamics of the pyridineâ€“acetylene hydrogen-bonded complex. Journal of Chemical Physics, 2015, 143, 104309.	1.2	9
95	Explicitly correlated ring-coupled-cluster-doubles theory. Journal of Chemical Physics, 2015, 142, 194106.	1.2	9
96	Highly Unsaturated Platinum and Palladium Carbenes PtC₃ and PdC₃ Isolated and Characterized in the Gas Phase. Angewandte Chemie - International Edition, 2016, 55, 3768-3771.	7.2	9
97	Insights on hydrogen bond assisted solvent selection in certain acidâ€“base heterogeneous catalysis through acceptor and donor numbers. Catalysis Science and Technology, 2021, 11, 1345-1357.	2.1	9
98	Probing computational methodologies in predicting mid-infrared spectra for large polycyclic aromatic hydrocarbons. Monthly Notices of the Royal Astronomical Society, 2022, 513, 3663-3681.	1.6	9
99	Interaction of a pseudo-Ï€ Câ€”C bond with cuprous and argentous chlorides: Cyclopropaneâ‹¯CuCl and cyclopropaneâ‹¯AgCl investigated by rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2015, 143, 164314.	1.2	8
100	Anharmonic Molecular Mechanics: Ab Initio Based Morse Parametrizations for the Popular MM3 Force Field. Journal of Physical Chemistry A, 2019, 123, 2991-2999.	1.1	8
101	Halogen Bonding in the Gas Phase: A Comparison of the Iodine Bond in Bâ‹¯ICl and Bâ‹¯ICF3 for Simple Lewis Bases B. Topics in Current Chemistry, 2014, 358, 43-77.	4.0	7
102	Quantum Yields for Photochemical Production of NO2 from Organic Nitrates at Tropospherically Relevant Wavelengths. Journal of Physical Chemistry A, 2014, 118, 2756-2764.	1.1	7
103	Cooperative hydrogen bonds form a pseudocycle stabilizing an isolated complex of isocyanic acid with urea. Physical Chemistry Chemical Physics, 2017, 19, 25080-25085.	1.3	6
104	Relaxing Constrained Amplitudes: Improved F12 Treatments of Orbital Optimization and Coreâ€“Valence Correlation Energies. Journal of Chemical Theory and Computation, 2018, 14, 5435-5440.	2.3	6
105	Computational study of the rovibrational spectrum of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e9065" altimg="si22.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>O-HF. Journal of Molecular Spectroscopy, 2022, 384, 111587.	0.4	6
106	Chemistry in Laser-Induced Plasmas: Formation of Mâ€“Câ‰¡Câ€“Cl (M = Ag or Cu) and their Characterization by Rotational Spectroscopy. Journal of Physical Chemistry A, 2015, 119, 2919-2925.	1.1	4
107	Zero-point energy and tunnelling: general discussion. Faraday Discussions, 2019, 221, 478-500.	1.6	4
108	A Structurally Characterized Fluoroalkyne. Angewandte Chemie, 2017, 129, 7659-7664.	1.6	3

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109	Anharmonic excited state frequencies of para-difluorobenzene, toluene and catechol using analytic RI-CC2 second derivatives. Physical Chemistry Chemical Physics, 2019, 21, 14063-14072.	1.3	3
110	Principal domains in F12 explicitly correlated theory. Advances in Quantum Chemistry, 2021, 83, 83-106.	0.4	3
111	The NosÃ©â€“Hoover looped chain thermostat for low temperature thawed Gaussian wave-packet dynamics. Journal of Chemical Physics, 2014, 140, 194106.	1.2	2
112	A Gaussian wave packet phase-space representation of quantum canonical statistics. Journal of Chemical Physics, 2015, 143, 044102.	1.2	2
113	Highly Unsaturated Platinum and Palladium Carbenes PtC₃ and PdC₃ Isolated and Characterized in the Gas Phase. Angewandte Chemie, 2016, 128, 3832-3835.	1.6	2
114	Noise resilience of Bayesian quantum phase estimation tested on a Si quantum photonic chip. , 2017, , .		2
115	Ground state solver on a silicon quantum photonic chip. , 2016, , .		0
116	The rotational spectrum of H₂Sâ‹¯HI and an investigation by ab initio calculations of the origins of the observed doubling of rotational transitions in both H₂Sâ‹¯HI and H₂Sâ‹¯F₂. Journal of Chemical Physics, 2020, 153, 204301.	1.2	0