Wesley D Allen

List of Publications by Citations

139 papers	10,424 citations	54 h-index	100 g-index
143 ext. papers	11,008 ext. citations	5.9 avg, IF	5.94 L-index

#	Paper	IF	Citations
139	Psi4: an open-source ab initio electronic structure program. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 556-565	7.9	678
138	In pursuit of the ab initio limit for conformational energy prototypes. *Journal of Chemical Physics*, **1998**, 108, 9751-9764	3.9	606
137	A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Asymmetric top molecules. *Chemical Physics*, **1988**, 123, 187-239	2.3	443
136	The C2H5 + O2 Reaction Mechanism: High-Level ab Initio Characterizations. *Journal of Physical Chemistry A*, **2000**, 104, 9823-9840	2.8	436
135	A hierarchy of homodesmotic reactions for thermochemistry. *Journal of the American Chemical Society*, **2009**, 131, 2547-60	16.4	418
134	The heat of formation of NCO. *Journal of Chemical Physics*, **1993**, 99, 4638-4650	3.9	335
133	Toward subchemical accuracy in computational thermochemistry: focal point analysis of the heat of formation of NCO and [H,N,C,O] isomers. *Journal of Chemical Physics*, **2004**, 120, 11586-99	3.9	285
132	A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules. *Chemical Physics*, **1990**, 145, 427-466	2.3	250
131	PSI3: an open-source Ab Initio electronic structure package. *Journal of Computational Chemistry*, **2007**, 28, 1610-1616	3.5	249
130	Coupling term derivation and general implementation of state-specific multireference coupled cluster theories. *Journal of Chemical Physics*, **2007**, 127, 024102	3.9	242
129	Capture of hydroxymethylene and its fast disappearance through tunnelling. *Nature*, **2008**, 453, 906-9	50.4	233
128	Methylhydroxycarbene: tunneling control of a chemical reaction. *Science*, **2011**, 332, 1300-3	33.3	226
127	Popular theoretical methods predict benzene and arenes to be nonplanar. *Journal of the American Chemical Society*, **2006**, 128, 9342-3	16.4	205
126	High-order excitations in state-universal and state-specific multireference coupled cluster theories: model systems. *Journal of Chemical Physics*, **2006**, 125, 154113	3.9	199
125	Definitive ab initio studies of model SN2 reactions CH(3)X+F- (X=F, Cl, CN, OH, SH, NH(2), PH(2)). *Chemistry - A European Journal*, **2003**, 9, 2173-92	4.8	185
124	On the ab initio determination of higher-order force constants at nonstationary reference geometries. *Journal of Chemical Physics*, **1993**, 98, 2983-3015	3.9	151
123	The torsional conformations of butane: Definitive energetics from ab initio methods. *Journal of Chemical Physics*, **1997**, 106, 5143-5150	3.9	145

122	Geometrical structures, force constants, and vibrational spectra of SiH, SiH2, SiH3, and SiH4. *Chemical Physics*, **1986**, 108, 243-274	2.3	142
121	Mechanism of the C2H5+O2 reaction. *Journal of Chemical Physics*, **1997**, 107, 141-155	3.9	137
120	Hartree□Fock orbital instability envelopes in highly correlated single-reference wave functions. *Journal of Chemical Physics*, **1997**, 107, 10626-10632	3.9	128
119	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	3.9	119
118	Is Mo/ller□Plesset perturbation theory a convergent ab initio method?. *Journal of Chemical Physics*, **2000**, 112, 9213-9222	3.9	117
117	Characterization of the X 1A□state of isocyanic acid. *Journal of Chemical Physics*, **1993**, 98, 1299-1328	3.9	116
116	Conformers of Gaseous Cysteine. *Journal of Chemical Theory and Computation*, **2009**, 5, 1511-23	6.4	111
115	The lithium superoxide radical: Symmetry breaking phenomena and potential energy surfaces. *Chemical Physics*, **1989**, 133, 11-45	2.3	111
114	Assessment of Density Functional Theory for Model SN2 Reactions:□CH3X + F-(X = F, Cl, CN, OH, SH, NH2, PH2). *Journal of Physical Chemistry A*, **2001**, 105, 11327-11346	2.8	107
113	The puckering inversion barrier and vibrational spectrum of cyclopentene. A scaled quantum mechanical force field algorithm. *Journal of the American Chemical Society*, **1992**, 114, 6834-6849	16.4	103
112	The analytic evaluation of energy first derivatives for two-configuration self-consistent-field configuration interaction (TCSCF-CI) wave functions. Application to ozone and ethylene. *Journal of Chemical Physics*, **1987**, 87, 7062-7075	3.9	102
111	The anharmonic force field and equilibrium molecular structure of ketene. *Journal of Chemical Physics*, **1995**, 102, 8506-8532	3.9	96
110	Exact ligand cone angles. *Journal of Computational Chemistry*, **2013**, 34, 1189-97	3.5	89
109	Ab Initio Anharmonic Vibrational Analyses of Non-Rigid Molecules **1993**, 343-373		80
108	Model identity SN2 reactions CH3X + X- (X = F, Cl, CN, OH, SH, NH2, PH2): Marcus theory analyzed. *Journal of Physical Chemistry A*, **2005**, 109, 10613-28	2.8	72
107	A high level ab initio map and direct statistical treatment of the fragmentation of singlet ketene. *Journal of Chemical Physics*, **1996**, 105, 118-140	3.9	72
106	Molecular structure of proline. *Chemistry - A European Journal*, **2004**, 10, 4512-7	4.8	71
105	The SN2 identity exchange reaction ClCH2CN + Cl- .fwdarw. Cl- + ClCH2CN: experiment and theory. *Journal of the American Chemical Society*, **1992**, 114, 9136-9153	16.4	71

104	Unimolecular thermal fragmentation of ortho-benzyne. *Journal of Chemical Physics*, **2007**, 126, 044312	3.9	70
103	Ionization thresholds of small carbon clusters: tunable VUV experiments and theory. *Journal of the American Chemical Society*, **2007**, 129, 10229-43	16.4	69
102	Analytic gradients for the state-specific multireference coupled cluster singles and doubles model. *Journal of Chemical Physics*, **2009**, 131, 064109	3.9	68
101	Molecular structures of the two most stable conformers of free glycine. *Journal of Computational Chemistry*, **2007**, 28, 1373-83	3.5	68
100	On the accuracy limits of orbital expansion methods: Explicit effects of k-functions on atomic and molecular energies. *Journal of Chemical Physics*, **2003**, 118, 8594-8610	3.9	68
99	The effect of 1s correlation on De, re, and ω of first-row diatomics. *Journal of Chemical Physics*, **1996**, 104, 2746-2748	3.9	67
98	The barrier to linearity of water. *Journal of Chemical Physics*, **1999**, 110, 11971-11981	3.9	65
97	Reactions between resonance-stabilized radicals: propargyl + allyl. *Journal of Physical Chemistry A*, **2010**, 114, 4881-90	2.8	64
96	Thermochemistry of disputed soot formation intermediates C4H3 and C4H5. *Journal of Chemical Physics*, **2004**, 121, 8800-13	3.9	64
95	Lowest-Lying Conformers of Alanine: Pushing Theory to Ascertain Precise Energetics and Semiexperimental Re Structures. *Journal of Chemical Theory and Computation*, **2010**, 6, 3066-78	6.4	63
94	Origin of the SN2 benzylic effect. *Journal of the American Chemical Society*, **2008**, 130, 9887-96	16.4	63
93	Downfield proton chemical shifts are not reliable aromaticity indicators. *Organic Letters*, **2005**, 7, 1457-60	6.2	62
92	Complete basis set limit studies of conventional and R12 correlation methods: The silicon dicarbide (SiC2) barrier to linearity. *Journal of Chemical Physics*, **2003**, 118, 7353	3.9	62
91	Reaction paths for the dissociation a 3A″ CH2CO-X̃ 3B1 CH2 + X 1Σ+ CO. *Journal of Chemical Physics*, **1988**, 89, 329-344	3.9	61
90	A companion perturbation theory for state-specific multireference coupled cluster methods. *Physical Chemistry Chemical Physics*, **2009**, 11, 4728-41	3.6	60
89	The highly anharmonic BH5 potential energy surface characterized in the ab initio limit. *Journal of Chemical Physics*, **2005**, 122, 104302	3.9	58
88	General derivative relations for anharmonic force fields. *Molecular Physics*, **1996**, 89, 1213-1221	1.7	58
87	The anharmonic force fields of HOF and F2O. *Journal of Chemical Physics*, **1988**, 89, 4965-4975	3.9	57

86	Assigning quantum labels to variationally computed rotational-vibrational eigenstates of polyatomic molecules. *Journal of Chemical Physics*, **2010**, 133, 034113	3.9	54
85	Thermochemistry of key soot formation intermediates: C3H3 isomers. *Journal of Physical Chemistry A*, **2007**, 111, 3819-30	2.8	54
84	Anharmonic force field, vibrational energies, and barrier to inversion of SiH3□ *Journal of Chemical Physics*, **2000**, 112, 4053-4063	3.9	52
83	Toward resolution of the silicon dicarbide (SiC2) saga: Ab initio excursions in the web of polytopism. *Journal of Chemical Physics*, **1997**, 107, 1195-1211	3.9	51
82	Ab initio studies of the low-lying electronic states of ketene. *Journal of Chemical Physics*, **1986**, 84, 2212-2225	3.9	51
81	The SN2 Identity Exchange Reaction F- + CH3F .fwdarw. FCH3 + F-: Definitive ab Initio Predictions. *The Journal of Physical Chemistry*, **1994**, 98, 13532-13540		50
80	The ab initio limit quartic force field of BH3. *Journal of Computational Chemistry*, **2005**, 26, 1106-12	3.5	49
79	Is the oxywater radical cation more stable than neutral oxywater?. *Journal of Chemical Physics*, **1996**, 104, 7615-7623	3.9	49
78	[5]Paracyclophane. An important example of ring strain and aromaticity in hydrocarbon compounds. *Journal of the American Chemical Society*, **1987**, 109, 2902-2909	16.4	49
77	Phenylhydroxycarbene. *Journal of the American Chemical Society*, **2010**, 132, 7273-5	16.4	48
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75	Dream or Reality: Complete Basis Set Full Configuration Interaction Potential Energy Hypersurfaces **2001**, 317-339		47
74	The infrared spectrum of the hydrogen bifluoride anion: unprecedented variation with level of theory. *Chemical Physics Letters*, **1986**, 131, 352-358	2.5	47
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72	On apparent quantized transition-state thresholds in the photofragmentation of acetaldehyde. *Journal of Chemical Physics*, **2000**, 112, 5585-5592	3.9	44
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70	Probing the Delicate Balance between Pauli Repulsion and London Dispersion with Triphenylmethyl Derivatives. *Journal of the American Chemical Society*, **2018**, 140, 14421-14432	16.4	43
69	An ab initio study of the vibrational spectrum of bicyclo[1.1.0]but-1(3)-ene. *Journal of the American Chemical Society*, **1987**, 109, 1615-1621	16.4	42

68	The Electronic Structure and Vibrational Spectrum oftrans-HNOO *Journal of Physical Chemistry A*, **2004**, 108, 2893-2903	2.8	40
67	Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices. *Journal of Computational Chemistry*, **2001**, 22, 1574-1589	3.5	40
66	Enthalpy of formation and anharmonic force field of diacetylene. *Journal of Chemical Physics*, **2009**, 130, 044301	3.9	39
65	Anchoring the Absolute Proton Affinity Scale. *Journal of Chemical Theory and Computation*, **2008**, 4, 1220-9	5.4	39
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62	Domino Tunneling. *Journal of the American Chemical Society*, **2015**, 137, 7828-34	16.4	36
61	A combined crossed-beam, ab initio, and RiceRamspergerKasselMarcus investigation of the reaction of carbon atoms C(3Pj) with benzene, C6H6(X 1A1g) and d6-benzene, C6D6(X 1A1g). *Journal of Chemical Physics*, **2002**, 116, 3248-3262	3.9	36
60	Benchmark configuration interaction spectroscopic constants for X 1+ C2 and X 1 CN+. *Journal of Chemical Physics*, **1998**, 108, 6717-6721	3.9	36
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56	Complexation in nickel-catalyzed cross-coupling reactions. *Journal of Organic Chemistry*, **2014**, 79, 1836-41	4.1	30
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47	Adsorbing Colloid Flotation of Cu(II) with a Chelating Surfactant. *Separation Science and Technology*, **1979**, 14, 769-776	2.5	25
46	Tunnelling in carbonic acid. *Chemical Communications*, **2016**, 52, 7858-61	5.8	24
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43	Nearly degenerate isomers of C(BH)2: cumulene, carbene, or carbone?. *Chemistry - A European Journal*, **2013**, 19, 15941-54	4.8	22
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38	Conformers of Gaseous Serine. *Journal of Chemical Theory and Computation*, **2016**, 12, 3571-82	6.4	20
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34	Exact Ligand Solid Angles. *Journal of Chemical Theory and Computation*, **2013**, 9, 5734-44	6.4	19
33	In search of definitive signatures of the elusive NCCO radical. *Journal of Chemical Physics*, **2007**, 127, 014306	3.9	19

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31	Secondary structures of peptides and proteins via NMR chemical-shielding anisotropy (CSA) parameters. *Journal of the American Chemical Society*, **2007**, 129, 1568-77	16.4	18
30	A first principles theoretical determination of the rate constant for the dissociation of singlet ketene. *Journal of Chemical Physics*, **1994**, 101, 9198-9201	3.9	18
29	Do π-conjugative effects facilitate SN2 reactions?. *Journal of the American Chemical Society*, **2014**, 136, 3118-26	16.4	17
28	Ring-Walking of Zerovalent Nickel on Aryl Halides. *Journal of Chemical Theory and Computation*, **2017**, 13, 1706-1711	6.4	15
27	On the convergence of Z-averaged perturbation theory. *Journal of Chemical Physics*, **2008**, 128, 074107	3.9	15
26	Interlocking Triplet Electronic States of Isocyanic Acid: Sources of Nonadiabatic Photofragmentation Dynamics. *Journal of Physical Chemistry A*, **2001**, 105, 2716-2730	2.8	14
25	The electronic structure of vanadium monochloride cation (VCl(+)): tackling the complexities of transition metal species. *Journal of Chemical Physics*, **2014**, 141, 204302	3.9	12
24	The multichannel n-propyl + O2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. *Journal of Chemical Physics*, **2018**, 148, 094303	3.9	11
23	Infrared signatures of the NCCO radical. *Physical Chemistry Chemical Physics*, **2009**, 11, 10385-90	3.6	11
22	Nucleophilic Influences and Origin of the S 2 Allylic Effect. *Chemistry - A European Journal*, **2018**, 24, 11637811648	4.8	10
21	Chemistry as a function of the fine-structure constant and the electron-proton mass ratio. *Physical Review A*, **2010**, 81,	2.6	10
20	The problematic C2H4+F2 reaction barrier. *Journal of Chemical Physics*, **2010**, 132, 094304	3.9	10
19	Tunneling Isomerizations on the Potential Energy Surfaces of Formaldehyde and Methanol Radical Cations. *ACS Earth and Space Chemistry*, **2017**, 1, 361-367	3.2	9
18	Intricate internal rotation surface and fundamental infrared transitions of the n-propyl radical. *Journal of Physical Chemistry B*, **2015**, 119, 728-35	3.4	9
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14	Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices **2001**, 22, 1574		7
13	Sub-Doppler infrared spectroscopy and formation dynamics of triacetylene in a slit supersonic expansion. *Journal of Chemical Physics*, **2016**, 144, 074301	3.9	6
12	Most favorable cumulenic structures in iron-capped linear carbon chains are short singlet odd-carbon dications: a theoretical view. *Physical Chemistry Chemical Physics*, **2018**, 20, 15496-15506	3.6	5
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9	Polytriangulane. *Journal of Chemical Theory and Computation*, **2016**, 12, 4707-16	6.4	4
8	Identification and Reactivity of -,--Dihydroxycarbene, a New [CHO] Intermediate. *Journal of the American Chemical Society*, **2020**, 142, 19457-19461	16.4	3
7	General derivative relations for anharmonic force fields		3
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5	The Li HF van der Waals minimum and the barrier to the deep HFi potential well Special Issue of Molecular Physics: Seventh Molecular Quantum Mechanics Conference, Lugano, Switzerland, 2 June 2013.View all notes. *Molecular Physics*, **2014**, 112, 770-773	1.7	2
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