Steven Gwaltney

List of Publications by Year
in descending order

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65 papers	8,509 citations	201385 27 h-index	123241 61 g-index
66 all docs	66 docs citations	66 times ranked	8701 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	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	1.5	617
4	Ground-state correlation energies for atomic ions with 3 to 18 electrons. Physical Review A, 1993, 47, 3649-3670.	1.0	488
5	A thermodynamic analysis of hydrogen production by steam reforming of glycerol. International Journal of Hydrogen Energy, 2007, 32, 2875-2880.	3.8	275
6	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
7	A second-order perturbative correction to the coupled-cluster singles and doubles method: CCSD(2). Journal of Chemical Physics, 2001, 115, 2014-2021.	1.2	154
8	Coupledâ€cluster calculations of the excitation energies of ethylene, butadiene, and cyclopentadiene. Journal of Chemical Physics, 1996, 105, 6979-6988.	1.2	141
9	A second-order correction to singles and doubles coupled-cluster methods based on a perturbative expansion of a similarity-transformed Hamiltonian. Chemical Physics Letters, 2000, 323, 21-28.	1.2	137
10	Simplified methods for equation-of-motion coupled-cluster excited state calculations. Chemical Physics Letters, 1996, 248, 189-198.	1.2	112
11	Coupled-cluster calculations of the electronic excitation spectrum of free base porphin in a polarized basis. Journal of Chemical Physics, 1998, 108, 6790-6798.	1.2	98
12	Charge-Transfer Mechanism for Electrophilic Aromatic Nitration and Nitrosation via the Convergence of (ab Initio) Molecular-Orbital and Marcusâ"Hush Theories with Experiments. Journal of the American Chemical Society, 2003, 125, 3273-3283.	6.6	88
13	A perturbative correction to the quadratic coupled-cluster doubles method for higher excitations. Chemical Physics Letters, 2002, 353, 359-367.	1.2	79
14	An application of the equation-of-motion coupled cluster method to the excited states of formaldehyde, acetaldehyde, and acetone. Chemical Physics Letters, 1995, 241, 26-32.	1.2	76
15	Approaching closed-shell accuracy for radicals using coupled cluster theory with perturbative triple substitutions. Physical Chemistry Chemical Physics, 2003, 5, 2488.	1.3	57
16	Interfacial shear strength of cured vinyl ester resin-graphite nanoplatelet from molecular dynamics simulations. Polymer, 2013, 54, 3282-3289.	1.8	57
17	Molecular dynamics simulations of vinyl ester resin monomer interactions with a pristine vapor-grown carbon nanofiber and their implications for composite interphase formation. Carbon, 2011, 49, 3219-3232.	5.4	53
18	Relative Reactivity Volume Criterion for Cross-Linking: Application to Vinyl Ester Resin Molecular Dynamics Simulations. Macromolecules, 2012, 45, 4876-4885.	2.2	45

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19	Transformation of Triclosan by Fe(III)-Saturated Montmorillonite. Environmental Science & Technology, 2010, 44, 668-674.	4.6	41
20	An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method. Physical Chemistry Chemical Physics, 2014, 16, 6233-6249.	1.3	41
21	Molecular dynamics simulations of oxidized vapor-grown carbon nanofiber surface interactions with vinyl ester resin monomers. Carbon, 2012, 50, 748-760.	5.4	40
22	Gradients for the partitioned equation-of-motion coupled-cluster method. Journal of Chemical Physics, 1999, 110, 62-71.	1.2	37
23	Gradients for the similarity transformed equation-of-motion coupled-cluster method. Journal of Chemical Physics, 1999, 111, 58-64.	1.2	34
24	Second-order correction to perfect pairing: An inexpensive electronic structure method for the treatment of strong electron-electron correlations. Journal of Chemical Physics, 2006, 124, 114107.	1.2	32
25	Structures and stabilities of copper encapsulated within silicon nano-clusters: Cu@Sin (n=9â€“15). Chemical Physics Letters, 2008, 451, 93-97.	1.2	31
26	Free volume and internal structural evolution during creep in model amorphous polyethylene by Molecular Dynamics simulations. Polymer, 2019, 170, 85-100.	1.8	30
27	Excitation Spectra of Dibenzoborole Containing Ï€-Electron Systems:â€‰ Controlling the Electronic Spectra by Changing the pÏ€â*Ï€* Conjugation. Journal of Physical Chemistry A, 2006, 110, 2434-2439.	1.1	28
28	Nanomechanics of phospholipid bilayer failure under strip biaxial stretching using molecular dynamics. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 055008.	0.8	28
29	Base Properties of H2CO in the Excited1nâ†'Ï€* State. Journal of Physical Chemistry A, 1998, 102, 5124-5127.	1.1	27
30	Calculating the equilibrium structure of the BNB molecule: Real Ã®Æ'Âµs. artifactual symmetry breaking. Physical Chemistry Chemical Physics, 2001, 3, 4495-4500.	1.3	27
31	Highâ€resolution zero kinetic energy photoelectron spectra of paraâ€nâ€propylaniline. Journal of Chemical Physics, 1994, 100, 5411-5421.	1.2	21
32	Evaluation of the â€˜side doorâ€™ in carboxylesterase-mediated catalysis and inhibition. Biological Chemistry, 2008, 389, 149-162.	1.2	20
33	Novel Nucleophiles Enhance the Human Serum Paraoxonase 1 (PON1)-mediated Detoxication of Organophosphates. Toxicological Sciences, 2015, 143, 46-53.	1.4	18
34	Interatomic Potential for Hydrocarbons on the Basis of the Modified Embedded-Atom Method with Bond Order (MEAM-BO). Journal of Physical Chemistry A, 2017, 121, 1502-1524.	1.1	18
35	New Design Strategy Toward NIR I Xanthene-Based Dyes. Journal of Organic Chemistry, 2020, 85, 12108-12116.	1.7	16
36	Thienylpiperidine Donor NIR Xanthene-Based Dye for Photoacoustic Imaging. Organic Letters, 2021, 23, 7640-7644.	2.4	15

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37	Can coupled cluster singles and doubles be approximated by a valence active space model?. Journal of Chemical Physics, 2002, 117, 3040-3048.	1.2	14
38	Determination of the stability constants for the binding of sulfonated morin with Fe2+. Inorganica Chimica Acta, 2007, 360, 2339-2344.	1.2	14
39	Simulations of tensile bond rupture in single alkane molecules using reactive interatomic potentials. Chemical Physics Letters, 2015, 635, 278-284.	1.2	14
40	Structure and dynamics of the S3 state of CS2. Journal of Chemical Physics, 1997, 107, 6570-6576.	1.2	11
41	Insertion of transition metal atoms and ions into the nanoscale dodecahedral silsesquioxane (T12-POSS) cage: Structures, stabilities and electronic properties. Chemical Physics Letters, 2009, 467, 348-353.	1.2	11
42	Global and local molecular dynamics of a bacterial carboxylesterase provide insight into its catalytic mechanism. Journal of Molecular Modeling, 2012, 18, 2869-2883.	0.8	11
43	Structures and Stabilities of the Metal Doped Gold Nano-Clusters: M@Au10 (MÂ=ÂW, Mo, Ru, Co). Journal of Inorganic and Organometallic Polymers and Materials, 2014, 24, 241-249.	1.9	11
44	Calculations of relative intensities of fragment ions in the MSMS spectra of a doubly charged penta-peptide. BMC Bioinformatics, 2012, 13, S13.	1.2	9
45	Effect of graphene dispersion on the equilibrium structure and deformation of graphene/eicosane composites as surrogates for graphene/polyethylene composites: a molecular dynamics simulation. Journal of Materials Science, 2017, 52, 5672-5685.	1.7	9
46	Molecular dynamics simulations showing 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) membrane mechanoporation damage under different strain paths. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1346-1359.	2.0	8
47	A nanoscale study of size scale, strain rate, temperature, and stress state effects on damage and fracture of polyethylene. Mechanics of Materials, 2021, 161, 104008.	1.7	7
48	Comment on: The relation between intensity and dipole moment for bending modes in linear molecules. Journal of Chemical Physics, 1993, 99, 3151-3152.	1.2	6
49	Coupled Cluster Methods for Bond-Breaking. ACS Symposium Series, 2002, , 93-108.	0.5	6
50	Behavior of protruding lateral plane graphene sheets in liquid dodecane: molecular dynamics simulations. Journal of Nanoparticle Research, 2016, 18, 1.	0.8	6
51	Isolation and structure of the anti,anti isomer and a DFT study ofÂitÂandÂthe syn,anti isomer of bis(tricarbonylchromium)dibenzo-[a,e]cyclooctatetraene. Evidence for an attractive electrostatic interaction between carbonyl oxygen atoms and Cr(CO)3-coordinated arene carbon atoms. Journal of Organometallic Chemistry, 2013, 745-746, 86-92.	0.8	5
52	NeON⁺: An Atom and a Molecule. ACS Earth and Space Chemistry, 2018, 2, 491-495.	1.2	5
53	Partitioning Techniques in Coupled-Cluster Theory. , 2003, , 433-457.		5
54	Molecular dynamics simulations of the graphene sheet aggregation in dodecane. Journal of Nanoparticle Research, 2017, 19, 1.	0.8	4

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55	Molecular dynamics simulations of the aggregation behaviour of overlapped graphene sheets in linear aliphatic hydrocarbons. Molecular Simulation, 2018, 44, 947-953.	0.9	4
56	Quantifying Parameter Sensitivity and Uncertainty for Interatomic Potential Design: Application to Saturated Hydrocarbons. ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering, 2018, 4, .	0.7	4
57	Dispersion-Corrected Modified Embedded-Atom Method Bond Order Interatomic Potential for Sulfur. Journal of Physical Chemistry A, 2018, 122, 9572-9578.	1.1	4
58	Cyclooctadiene Rh(I) Bis- and Tris(pyrazolyl)aluminate Complexes and Their Catalytic Activity on the Polymerization of Phenylacetylene. Inorganic Chemistry, 2021, 60, 10757-10763.	1.9	4
59	SMALL PURE CARBON MOLECULES WITH SMALL-WORLD NETWORKS USING DENSITY FUNCTIONAL THEORY SIMULATIONS. International Journal of Modern Physics C, 2009, 20, 1345-1356.	0.8	2
60	A theoretical analysis of substituted aromatic compounds. International Journal of Quantum Chemistry, 2013, 113, 1171-1179.	1.0	2
61	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
62	The Role of Mutations at the Side Door on the Thermal Stability and Structural Flexibility of the pnbCE Enzyme. Zeitschrift Fur Physikalische Chemie, 2016, 230, 837-849.	1.4	1
63	Single-wall carbon nanotube mechanical behavior using the modified embedded atom method with bond order (MEAM-BO). Modelling and Simulation in Materials Science and Engineering, 0, , .	0.8	1
64	Using Histone H1 Derived Peptides to Investigate Binding Affinity and Inter-Domain Dynamics in Human Pin1. Biophysical Journal, 2019, 116, 463a.	0.2	0
65	Structure and Energetics of Polyhedral Oligomeric Silsesquioxane (T8,T10,T12-POSS) Cages with Atomic and Ionic Lithium Species. , 2014, , 151-165.		0