

Steven Gwaltney

List of Publications by Year in descending order

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65
papers

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201385

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docs citations

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8701
citing authors

#	ARTICLE	IF	CITATIONS
1	Cyclooctadiene Rh(I) Bis- and Tris(pyrazolyl)aluminate Complexes and Their Catalytic Activity on the Polymerization of Phenylacetylene. <i>Inorganic Chemistry</i> , 2021, 60, 10757-10763.	1.9	4
2	Thienylpiperidine Donor NIR Xanthene-Based Dye for Photoacoustic Imaging. <i>Organic Letters</i> , 2021, 23, 7640-7644.	2.4	15
3	A nanoscale study of size scale, strain rate, temperature, and stress state effects on damage and fracture of polyethylene. <i>Mechanics of Materials</i> , 2021, 161, 104008.	1.7	7
4	New Design Strategy Toward NIR I Xanthene-Based Dyes. <i>Journal of Organic Chemistry</i> , 2020, 85, 12108-12116.	1.7	16
5	Using Histone H1 Derived Peptides to Investigate Binding Affinity and Inter-Domain Dynamics in Human Pin1. <i>Biophysical Journal</i> , 2019, 116, 463a.	0.2	0
6	Free volume and internal structural evolution during creep in model amorphous polyethylene by Molecular Dynamics simulations. <i>Polymer</i> , 2019, 170, 85-100.	1.8	30
7	Molecular dynamics simulations showing 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) membrane mechanoporation damage under different strain paths. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 1346-1359.	2.0	8
8	Molecular dynamics simulations of the aggregation behaviour of overlapped graphene sheets in linear aliphatic hydrocarbons. <i>Molecular Simulation</i> , 2018, 44, 947-953.	0.9	4
9	NeON ⁺ : An Atom and a Molecule. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 491-495.	1.2	5
10	Quantifying Parameter Sensitivity and Uncertainty for Interatomic Potential Design: Application to Saturated Hydrocarbons. <i>ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering</i> , 2018, 4, .	0.7	4
11	Dispersion-Corrected Modified Embedded-Atom Method Bond Order Interatomic Potential for Sulfur. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9572-9578.	1.1	4
12	Interatomic Potential for Hydrocarbons on the Basis of the Modified Embedded-Atom Method with Bond Order (MEAM-BO). <i>Journal of Physical Chemistry A</i> , 2017, 121, 1502-1524.	1.1	18
13	Effect of graphene dispersion on the equilibrium structure and deformation of graphene/eicosane composites as surrogates for graphene/polyethylene composites: a molecular dynamics simulation. <i>Journal of Materials Science</i> , 2017, 52, 5672-5685.	1.7	9
14	Molecular dynamics simulations of the graphene sheet aggregation in dodecane. <i>Journal of Nanoparticle Research</i> , 2017, 19, 1.	0.8	4
15	Nanomechanics of phospholipid bilayer failure under strip biaxial stretching using molecular dynamics. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016, 24, 055008.	0.8	28
16	The Role of Mutations at the Side Door on the Thermal Stability and Structural Flexibility of the pnbCE Enzyme. <i>Zeitschrift Fur Physikalische Chemie</i> , 2016, 230, 837-849.	1.4	1
17	Behavior of protruding lateral plane graphene sheets in liquid dodecane: molecular dynamics simulations. <i>Journal of Nanoparticle Research</i> , 2016, 18, 1.	0.8	6
18	Simulations of tensile bond rupture in single alkane molecules using reactive interatomic potentials. <i>Chemical Physics Letters</i> , 2015, 635, 278-284.	1.2	14

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19	Novel Nucleophiles Enhance the Human Serum Paraoxonase 1 (PON1)-mediated Detoxication of Organophosphates. <i>Toxicological Sciences</i> , 2015, 143, 46-53.	1.4	18
20	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
21	Structures and Stabilities of the Metal Doped Gold Nano-Clusters: M@Au ₁₀ (M=Ag, Au, Cu, Ni, Pt, Pd, Mo, Ru, Co). <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2014, 24, 241-249.	1.9	11
22	An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6233-6249.	1.3	41
23	Structure and Energetics of Polyhedral Oligomeric Silsesquioxane (T ₈ , T ₁₀ , T ₁₂ -POSS) Cages with Atomic and Ionic Lithium Species. , 2014, , 151-165.		0
24	A theoretical analysis of substituted aromatic compounds. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1171-1179.	1.0	2
25	Isolation and structure of the anti,anti isomer and a DFT study of the 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. <i>Journal of Organometallic Chemistry</i> , 2013, 745-746, 86-92.	0.8	5
26	Interfacial shear strength of cured vinyl ester resin-graphite nanoplatelet from molecular dynamics simulations. <i>Polymer</i> , 2013, 54, 3282-3289.	1.8	57
27	Relative Reactivity Volume Criterion for Cross-Linking: Application to Vinyl Ester Resin Molecular Dynamics Simulations. <i>Macromolecules</i> , 2012, 45, 4876-4885.	2.2	45
28	Calculations of relative intensities of fragment ions in the MSMS spectra of a doubly charged penta-peptide. <i>BMC Bioinformatics</i> , 2012, 13, S13.	1.2	9
29	Global and local molecular dynamics of a bacterial carboxylesterase provide insight into its catalytic mechanism. <i>Journal of Molecular Modeling</i> , 2012, 18, 2869-2883.	0.8	11
30	Molecular dynamics simulations of oxidized vapor-grown carbon nanofiber surface interactions with vinyl ester resin monomers. <i>Carbon</i> , 2012, 50, 748-760.	5.4	40
31	Molecular dynamics simulations of vinyl ester resin monomer interactions with a pristine vapor-grown carbon nanofiber and their implications for composite interphase formation. <i>Carbon</i> , 2011, 49, 3219-3232.	5.4	53
32	Transformation of Triclosan by Fe(III)-Saturated Montmorillonite. <i>Environmental Science & Technology</i> , 2010, 44, 668-674.	4.6	41
33	SMALL PURE CARBON MOLECULES WITH SMALL-WORLD NETWORKS USING DENSITY FUNCTIONAL THEORY SIMULATIONS. <i>International Journal of Modern Physics C</i> , 2009, 20, 1345-1356.	0.8	2
34	Insertion of transition metal atoms and ions into the nanoscale dodecahedral silsesquioxane (T ₁₂ -POSS) cage: Structures, stabilities and electronic properties. <i>Chemical Physics Letters</i> , 2009, 467, 348-353.	1.2	11
35	Structures and stabilities of copper encapsulated within silicon nano-clusters: Cu@Si _n (n=9-15). <i>Chemical Physics Letters</i> , 2008, 451, 93-97.	1.2	31
36	Evaluation of the "side door"™ in carboxylesterase-mediated catalysis and inhibition. <i>Biological Chemistry</i> , 2008, 389, 149-162.	1.2	20

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37	Determination of the stability constants for the binding of sulfonated morin with Fe ²⁺ . <i>Inorganica Chimica Acta</i> , 2007, 360, 2339-2344.	1.2	14
38	A thermodynamic analysis of hydrogen production by steam reforming of glycerol. <i>International Journal of Hydrogen Energy</i> , 2007, 32, 2875-2880.	3.8	275
39	Second-order correction to perfect pairing: An inexpensive electronic structure method for the treatment of strong electron-electron correlations. <i>Journal of Chemical Physics</i> , 2006, 124, 114107.	1.2	32
40	Excitation Spectra of Dibenzoborole Containing π -Electron Systems: Controlling the Electronic Spectra by Changing the π - π^* Conjugation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2434-2439.	1.1	28
41	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	1.3	2,597
42	Approaching closed-shell accuracy for radicals using coupled cluster theory with perturbative triple substitutions. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 2488.	1.3	57
43	Charge-Transfer Mechanism for Electrophilic Aromatic Nitration and Nitrosation via the Convergence of (ab Initio) Molecular-Orbital and Marcus-Hush Theories with Experiments. <i>Journal of the American Chemical Society</i> , 2003, 125, 3273-3283.	6.6	88
44	Partitioning Techniques in Coupled-Cluster Theory. , 2003, , 433-457.		5
45	Can coupled cluster singles and doubles be approximated by a valence active space model?. <i>Journal of Chemical Physics</i> , 2002, 117, 3040-3048.	1.2	14
46	Coupled Cluster Methods for Bond-Breaking. <i>ACS Symposium Series</i> , 2002, , 93-108.	0.5	6
47	A perturbative correction to the quadratic coupled-cluster doubles method for higher excitations. <i>Chemical Physics Letters</i> , 2002, 353, 359-367.	1.2	79
48	Calculating the equilibrium structure of the BNB molecule: Real \tilde{A}^{∞} artifactual symmetry breaking. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 4495-4500.	1.3	27
49	A second-order perturbative correction to the coupled-cluster singles and doubles method: CCSD(2). <i>Journal of Chemical Physics</i> , 2001, 115, 2014-2021.	1.2	154
50	Q-Chem 2.0: a high-performance ab initio electronic structure program package. <i>Journal of Computational Chemistry</i> , 2000, 21, 1532-1548.	1.5	617
51	A second-order correction to singles and doubles coupled-cluster methods based on a perturbative expansion of a similarity-transformed Hamiltonian. <i>Chemical Physics Letters</i> , 2000, 323, 21-28.	1.2	137
52	Second-order perturbation corrections to singles and doubles coupled-cluster methods: General theory and application to the valence optimized doubles model. <i>Journal of Chemical Physics</i> , 2000, 113, 3548-3560.	1.2	155
53	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
54	Gradients for the similarity transformed equation-of-motion coupled-cluster method. <i>Journal of Chemical Physics</i> , 1999, 111, 58-64.	1.2	34

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55	Gradients for the partitioned equation-of-motion coupled-cluster method. <i>Journal of Chemical Physics</i> , 1999, 110, 62-71.	1.2	37
56	Base Properties of H ₂ CO in the Excited $1n\pi^*$ State. <i>Journal of Physical Chemistry A</i> , 1998, 102, 5124-5127.	1.1	27
57	Coupled-cluster calculations of the electronic excitation spectrum of free base porphin in a polarized basis. <i>Journal of Chemical Physics</i> , 1998, 108, 6790-6798.	1.2	98
58	Structure and dynamics of the S ₃ state of CS ₂ . <i>Journal of Chemical Physics</i> , 1997, 107, 6570-6576.	1.2	11
59	Coupled-cluster calculations of the excitation energies of ethylene, butadiene, and cyclopentadiene. <i>Journal of Chemical Physics</i> , 1996, 105, 6979-6988.	1.2	141
60	Simplified methods for equation-of-motion coupled-cluster excited state calculations. <i>Chemical Physics Letters</i> , 1996, 248, 189-198.	1.2	112
61	An application of the equation-of-motion coupled cluster method to the excited states of formaldehyde, acetaldehyde, and acetone. <i>Chemical Physics Letters</i> , 1995, 241, 26-32.	1.2	76
62	High-resolution zero kinetic energy photoelectron spectra of para-propylaniline. <i>Journal of Chemical Physics</i> , 1994, 100, 5411-5421.	1.2	21
63	Ground-state correlation energies for atomic ions with 3 to 18 electrons. <i>Physical Review A</i> , 1993, 47, 3649-3670.	1.0	488
64	Comment on: The relation between intensity and dipole moment for bending modes in linear molecules. <i>Journal of Chemical Physics</i> , 1993, 99, 3151-3152.	1.2	6
65	Single-wall carbon nanotube mechanical behavior using the modified embedded atom method with bond order (MEAM-BO). <i>Modelling and Simulation in Materials Science and Engineering</i> , 0, , .	0.8	1