David J Henry

List of Publications by Year
in descending order

71	2,131	257101	233125
papers	citations	24 h-index	45 g-index

72	72	72	1753
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	G3-RAD and G3X-RAD: Modified Gaussian-3 (G3) and Gaussian-3X (G3X) procedures for radical thermochemistry. Journal of Chemical Physics, 2003, 118, 4849-4860.	1.2	276
2	Bond Dissociation Energies and Radical Stabilization Energies Associated with Substituted Methyl Radicals. Journal of Physical Chemistry A, 2001, 105, 6750-6756.	1.1	265
3	Reliable Theoretical Procedures for Calculating the Rate of Methyl Radical Addition to Carbonâ^'Carbon Double and Triple Bonds. Journal of Physical Chemistry A, 2004, 108, 2874-2883.	1.1	122
4	An Assessment of the Performance of High-Level Theoretical Procedures in the Computation of the Heats of Formation of Small Open-Shell Molecules. Journal of Physical Chemistry A, 2002, 106, 7927-7936.	1.1	109
5	Effect of Substituents on Radical Stability in Reversible Addition Fragmentation Chain Transfer Polymerization:Â An ab Initio Study. Macromolecules, 2005, 38, 1415-1433.	2.2	92
6	Comparison of the Kinetics and Thermodynamics for Methyl Radical Addition to CC, CO, and CS Double Bonds. Journal of the American Chemical Society, 2004, 126, 1732-1740.	6.6	70
7	Performance of Numerical Basis Set DFT for Aluminum Clusters. Journal of Physical Chemistry A, 2008, 112, 9835-9844.	1.1	66
8	Effect of substituents on the stabilities of multiply-substituted carbon-centered radicals. Organic and Biomolecular Chemistry, 2011, 9, 3636.	1.5	63
9	Dissociative Adsorption of Hydrogen Molecule on Aluminum Clusters: Effect of Charge and Doping. Journal of Physical Chemistry A, 2009, 113, 2565-2571.	1.1	59
10	Alkoxy radicals in the gaseous phase: Î²-scission reactions and formation by radical addition to carbonyl compounds. Canadian Journal of Chemistry, 2003, 81, 431-442.	0.6	58
11	Computer-Aided Design of a Destabilized RAFT Adduct Radical:Â Toward Improved RAFT Agents for Styrene-block-Vinyl Acetate Copolymers. Macromolecules, 2005, 38, 5774-5779.	2.2	57
12	What Is the Origin of the Contrathermodynamic Behavior in Methyl Radical Addition to Alkynes versus Alkenes?. Journal of Physical Chemistry A, 2003, 107, 6082-6090.	1.1	43
13	Adhesion between Graphite and Modified Polyester Surfaces:Â A Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 17224-17231.	1.2	38
14	Organostannanes Derived from (â^')-Menthol:â€‰ Controlling Stereochemistry during the Preparation of (1R,2S,5R)-Menthyldiphenyltin Hydride and Bis((1R,2S,5R)-menthyl)phenyltin Hydride. Organometallics, 1999, 18, 3342-3347.	1.1	37
15	Performance of the RB3-LYP, RMP2, and UCCSD(T) Procedures in Calculating Radical Stabilization Energies for â€¢NHX Radicals. Journal of Physical Chemistry A, 2003, 107, 7985-7990.	1.1	37
16	Alginate Biopolymer Effect on the Electrodeposition of Manganese Dioxide on Electrodes for Supercapacitors. ACS Applied Energy Materials, 2021, 4, 7040-7051.	2.5	37
17	Monolayer Structure and Evaporation Resistance: A Molecular Dynamics Study of Octadecanol on Water. Journal of Physical Chemistry B, 2010, 114, 3869-3878.	1.2	36
18	Eucalyptus reforestation induces soil water repellency. Soil Research, 2015, 53, 168.	0.6	36

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19	First Principles Investigation of H Addition and Abstraction Reactions on Doped Aluminum Clusters. Journal of Physical Chemistry A, 2009, 113, 5832-5837.	1.1	34
20	DFT Study of H Adsorption on Magnesium-Doped Aluminum Clusters. Journal of Physical Chemistry A, 2010, 114, 3602-3608.	1.1	34
21	Novel Approach for Fabricating Transparent and Conducting SWCNTs/ITO Thin Films for Optoelectronic Applications. Journal of Physical Chemistry C, 2018, 122, 3014-3027.	1.5	33
22	Interpreting the near-infrared reflectance of a series of perylene pigments. Dyes and Pigments, 2013, 99, 502-511.	2.0	29
23	Theoretical study of adhesion between graphite, polyester and silica surfaces. Molecular Simulation, 2005, 31, 449-455.	0.9	27
24	Simulations of Nanoindentation of Polymer Surfaces: Effects of Surface Cross-Linking on Adhesion and Hardness. Journal of Physical Chemistry C, 2010, 114, 478-486.	1.5	27
25	Classical Molecular Dynamics Study of [60]Fullerene Interactions with Silica and Polyester Surfaces. Journal of Physical Chemistry B, 2006, 110, 15963-15972.	1.2	23
26	Reactivity and Regioselectivity of Aluminum Nanoclusters: Insights from Regional Density Functional Theory. Journal of Physical Chemistry C, 2011, 115, 1714-1723.	1.5	22
27	Comparative Study of Commonly Used Molecular Dynamics Force Fields for Modeling Organic Monolayers on Water. Journal of Physical Chemistry B, 2011, 115, 3964-3971.	1.2	22
28	Improved mechanical properties of sol-gel derived ITO thin films via Ag doping. Materials Today Communications, 2018, 14, 210-224.	0.9	21
29	Stannanes as free-radical reducing agents: an ab initio study of hydrogen atom transfer from some trialkyltin hydrides to alkyl radicals. Journal of the Chemical Society Perkin Transactions II, 1997, , 1665-1670.	0.9	20
30	Inhibition of Peptidylglycine Î±-Amidating Monooxygenase by Exploitation of Factors Affecting the Stability and Ease of Formation of Glycyl Radicals. Journal of the American Chemical Society, 2004, 126, 13306-13311.	6.6	20
31	Soil water repellency: A molecular-level perspective of a global environmental phenomenon. Geoderma, 2019, 338, 56-66.	2.3	19
32	Sol-gel derived ITO-based bi-layer and tri-layer thin film coatings for organic solar cells applications. Applied Surface Science, 2020, 530, 147164.	3.1	19
33	Carbohydrate coated fluorescent mesoporous silica particles for bacterial imaging. Colloids and Surfaces B: Biointerfaces, 2020, 188, 110751.	2.5	18
34	Effect of Surface Composition and Atomic Roughness on Interfacial Adhesion between Polyester and Amorphous Carbon. Journal of Physical Chemistry C, 2007, 111, 3000-3009.	1.5	17
35	Probing the effects of thermal treatment on the electronic structure and mechanical properties of Ti-doped ITO thin films. Journal of Alloys and Compounds, 2017, 721, 333-346.	2.8	16
36	Improving the optoelectronic properties of titanium-doped indium tin oxide thin films. Semiconductor Science and Technology, 2017, 32, 065011.	1.0	14

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37	Equilibria in Free-Radical Chemistry:Â An Ab Initio Study of Hydrogen Atom Transfer Reactions between Silyl, Germyl, and Stannyl Radicals and Their Hydrides. Organometallics, 1998, 17, 1079-1084.	1.1	12
38	Comb polymers: Are they the answer to monolayer stability?. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2011, 384, 482-489.	2.3	12
39	Structures and Stability of Doped Gallium Nanoclusters. Journal of Physical Chemistry C, 2012, 116, 24814-24823.	1.5	12
40	Stability and electronic structures of double-walled armchair germanium carbide nanotubes. Computational Materials Science, 2016, 111, 86-90.	1.4	11
41	Why do biogenic volatile organic compounds (BVOCs) derived from vegetation fire not induce soil water repellency?. Biogeochemistry, 2017, 134, 147-161.	1.7	11
42	Silanes and germanes as free-radical reducing agents: an ab initio study of hydrogen atom transfer from some trialkylsilanes and germanes to alkyl radicals. Journal of the Chemical Society Perkin Transactions II, 1998, , 591-602.	0.9	10
43	Steric trends and kinetic parameters for radical reductions involving alkyldiphenyltin hydrides. Journal of Physical Organic Chemistry, 1999, 12, 233-239.	0.9	10
44	Molecular Dynamics Study of Polyester Surfaces and Fullerene Particles in Aqueous Environment. Journal of Physical Chemistry C, 2008, 112, 18141-18149.	1.5	10
45	Effect of Substrate on the Mechanical Response and Adhesion of PEGylated Surfaces: Insights from All-Atom Simulations. Langmuir, 2012, 28, 17263-17272.	1.6	10
46	Hydrogen Adsorption on Gallium Nanoclusters. Journal of Physical Chemistry C, 2013, 117, 26269-26279.	1.5	10
47	Surface crosslinking effects on contamination resistance of functionalised polymers. Soft Matter, 2013, 9, 1798-1806.	1.2	9
48	Mechanism for the deamination of ammeline, guanine, and their analogues. Structural Chemistry, 2017, 28, 1467-1477.	1.0	9
49	Rethinking soil water repellency and its management. Plant Ecology, 2019, 220, 977-984.	0.7	8
50	Effect of Aging on Interfacial Adhesion between Polyester and Carbon-Based Particles:â€‰ A Classical Molecular Dynamics Study. Journal of Physical Chemistry C, 2007, 111, 6465-6472.	1.5	7
51	Homoanomeric Effect in the 1,2-Dimethoxyethyl Radical. Australian Journal of Chemistry, 2003, 56, 429.	0.5	6
52	Comparison of embedded atom method potentials for small aluminium cluster simulations. Journal of Physics Condensed Matter, 2009, 21, 144206.	0.7	6
53	Mechanistic investigation of halopentaaquachromium(III) complexes: Comparison of computational and experimental results. Computational and Theoretical Chemistry, 2015, 1070, 152-161.	1.1	6
54	Mechanistic study of the aquation of nutritional supplement chromium chloride and other chromium(III) dihalides. Computational and Theoretical Chemistry, 2016, 1084, 88-97.	1.1	5

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55	Investigation of the Spectroscopic, Thermal and Electrochemical Properties of Tris-(glycinato)chromium(III). ChemistrySelect, 2017, 2, 1950-1958.	0.7	5
56	Contribution of Binary Organic Layers to Soil Water Repellency: A Molecular Level Perspective. Journal of Physical Chemistry A, 2019, 123, 7518-7527.	1.1	5
57	Induction of water repellency by leaves of contrasting Australian native species: effects of composition and heating. Plant and Soil, 2022, 478, 505-517.	1.8	5
58	Calculated bond dissociation energies and enthalpy of formation of Î±-amino acid radicals. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	4
59	Layer effects on electronic structures of multi-walled armchair silicon carbide nanotubes. Computational Materials Science, 2016, 125, 117-122.	1.4	4
60	Further Theoretical Studies of the Aquation of Chromium(III) Chloride Nutritional Supplement: Effect of pH and Solvation. ChemistrySelect, 2016, 1, 5236-5249.	0.7	4
61	Hydrolytic deamination reactions of amidine and nucleobase derivatives. International Journal of Quantum Chemistry, 2020, 120, e26059.	1.0	4
62	Regional DFTâ€"Electronic Stress Tensor Study of Aluminum Nanostructures for Hydrogen Storage. , 2009, , .		3
63	Role of Hydrogen in Dimerizaton of Aluminum Clusters: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 7734-7743.	1.1	3
64	Is There Ni in My Liquor? A Hands-On Laboratory Exercise for Relating Chemistry to Extractive Metallurgy. Journal of Chemical Education, 2013, 90, 1671-1674.	1.1	3
65	Synthesis and characterization of novel silane derivatives of phenothiazinium photosensitisers. Dyes and Pigments, 2022, 199, 110087.	2.0	3
66	A molecular dynamics study of siloxane diffusion in a polyesterâ€"melamine solution. Polymer, 2007, 48, 2179-2185.	1.8	2
67	Quantification of deep soil carbon by a wet digestion technique. Soil Research, 2017, 55, 78.	0.6	2
68	Bonding in doped gallium nanoclusters: Insights from regional DFT. Computational Materials Science, 2016, 115, 145-153.	1.4	1
69	Investigation of mono-, bis- and tris-glycinatochromium(III): Comparisons of computational and experimental results. Polyhedron, 2017, 130, 81-93.	1.0	1
70	Theoretical Thermochemistry of Radicals. , 2001, , 161-197.		1
71	Ligand coordination effects on gallium nanocluster reactivity. Advanced Materials Letters, 2017, 8, 862-865.	0.3	0