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	Synthesis and characterization of novel silane derivatives of phenothiazinium photosensitisers. Dyes and Pigments, 2022, 199, 110087.	2.0	3
2	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
3	Alginate Biopolymer Effect on the Electrodeposition of Manganese Dioxide on Electrodes for Supercapacitors. ACS Applied Energy Materials, 2021, 4, 7040-7051.	2.5	37
4	Hydrolytic deamination reactions of amidine and nucleobase derivatives. International Journal of Quantum Chemistry, 2020, 120, e26059.	1.0	4
5	Carbohydrate coated fluorescent mesoporous silica particles for bacterial imaging. Colloids and Surfaces B: Biointerfaces, 2020, 188, 110751.	2.5	18
6	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
7	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
8	Rethinking soil water repellency and its management. Plant Ecology, 2019, 220, 977-984.	0.7	8
9	Soil water repellency: A molecular-level perspective of a global environmental phenomenon. Geoderma, 2019, 338, 56-66.	2.3	19
10	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
11	Improved mechanical properties of sol-gel derived ITO thin films via Ag doping. Materials Today Communications, 2018, 14, 210-224.	0.9	21
12	Mechanism for the deamination of ammeline, guanine, and their analogues. Structural Chemistry, 2017, 28, 1467-1477.	1.0	9
13	Investigation of mono-, bis- and tris-glycinatochromium(III): Comparisons of computational and experimental results. Polyhedron, 2017, 130, 81-93.	1.0	1
14	Improving the optoelectronic properties of titanium-doped indium tin oxide thin films. Semiconductor Science and Technology, 2017, 32, 065011.	1.0	14
15	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
16	Investigation of the Spectroscopic, Thermal and Electrochemical Properties of Tris-(glycinato)chromium(III). ChemistrySelect, 2017, 2, 1950-1958.	0.7	5
17	Quantification of deep soil carbon by a wet digestion technique. Soil Research, 2017, 55, 78.	0.6	2
18	Why do biogenic volatile organic compounds (BVOCs) derived from vegetation fire not induce soil water repellency?. Biogeochemistry, 2017, 134, 147-161.	1.7	11

#	Article	IF	Citations
19	Ligand coordination effects on gallium nanocluster reactivity. Advanced Materials Letters, 2017, 8, 862-865.	0.3	0
20	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
21	Calculated bond dissociation energies and enthalpy of formation of Î±-amino acid radicals. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	4
22	Layer effects on electronic structures of multi-walled armchair silicon carbide nanotubes. Computational Materials Science, 2016, 125, 117-122.	1.4	4
23	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
24	Bonding in doped gallium nanoclusters: Insights from regional DFT. Computational Materials Science, 2016, 115, 145-153.	1.4	1
25	Stability and electronic structures of double-walled armchair germanium carbide nanotubes. Computational Materials Science, 2016, 111, 86-90.	1.4	11
26	Eucalyptus reforestation induces soil water repellency. Soil Research, 2015, 53, 168.	0.6	36
27	Mechanistic investigation of halopentaaquachromium(III) complexes: Comparison of computational and experimental results. Computational and Theoretical Chemistry, 2015, 1070, 152-161.	1.1	6
28	Hydrogen Adsorption on Gallium Nanoclusters. Journal of Physical Chemistry C, 2013, 117, 26269-26279.	1.5	10
29	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
30	Surface crosslinking effects on contamination resistance of functionalised polymers. Soft Matter, 2013, 9, 1798-1806.	1.2	9
31	Interpreting the near-infrared reflectance of a series of perylene pigments. Dyes and Pigments, 2013, 99, 502-511.	2.0	29
32	Structures and Stability of Doped Gallium Nanoclusters. Journal of Physical Chemistry C, 2012, 116, 24814-24823.	1.5	12
33	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
34	Reactivity and Regioselectivity of Aluminum Nanoclusters: Insights from Regional Density Functional Theory. Journal of Physical Chemistry C, 2011, 115, 1714-1723.	1.5	22
35	Role of Hydrogen in Dimerizaton of Aluminum Clusters: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 7734-7743.	1.1	3
36	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

#	Article	IF	Citations
37	Effect of substituents on the stabilities of multiply-substituted carbon-centered radicals. Organic and Biomolecular Chemistry, 2011, 9, 3636.	1.5	63
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	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
40	DFT Study of H Adsorption on Magnesium-Doped Aluminum Clusters. Journal of Physical Chemistry A, 2010, 114, 3602-3608.	1.1	34
41	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
42	Comparison of embedded atom method potentials for small aluminium cluster simulations. Journal of Physics Condensed Matter, 2009, 21, 144206.	0.7	6
43	Regional DFTâ€"Electronic Stress Tensor Study of Aluminum Nanostructures for Hydrogen Storage. , 2009, , .		3
44	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
45	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
46	Performance of Numerical Basis Set DFT for Aluminum Clusters. Journal of Physical Chemistry A, 2008, 112, 9835-9844.	1.1	66
47	Molecular Dynamics Study of Polyester Surfaces and Fullerene Particles in Aqueous Environment. Journal of Physical Chemistry C, 2008, 112, 18141-18149.	1.5	10
48	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
49	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
50	A molecular dynamics study of siloxane diffusion in a polyesterâ€"melamine solution. Polymer, 2007, 48, 2179-2185.	1.8	2
51	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
52	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
53	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
54	Theoretical study of adhesion between graphite, polyester and silica surfaces. Molecular Simulation, 2005, 31, 449-455.	0.9	27

#	Article	IF	Citations
55	Adhesion between Graphite and Modified Polyester Surfaces:Â A Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 17224-17231.	1.2	38
56	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
57	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
58	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
59	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
60	Homoanomeric Effect in the 1,2-Dimethoxyethyl Radical. Australian Journal of Chemistry, 2003, 56, 429.	0.5	6
61	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
62	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
63	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
64	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
65	Bond Dissociation Energies and Radical Stabilization Energies Associated with Substituted Methyl Radicals. Journal of Physical Chemistry A, 2001, 105, 6750-6756.	1.1	265
66	Theoretical Thermochemistry of Radicals. , 2001, , 161-197.		1
67	Steric trends and kinetic parameters for radical reductions involving alkyldiphenyltin hydrides. Journal of Physical Organic Chemistry, 1999, 12, 233-239.	0.9	10
68	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
69	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
70	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
71	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