Daniel S Levine

List of Publications by Year
in descending order

28 papers	1,728 citations	331259 21 h-index	500791 28 g-index
28 all docs	28 docs citations	28 times ranked	1772 citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
2	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	2.1	90
3	Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method. Journal of Chemical Theory and Computation, 2020, 16, 2139-2159.	2.3	90
4	Isolation of Pure Disubstituted E Olefins through Mo-Catalyzed Z-Selective Ethenolysis of Stereoisomeric Mixtures. Journal of the American Chemical Society, 2011, 133, 11512-11514.	6.6	87
5	Expanded Helicenes: A General Synthetic Strategy and Remarkable Supramolecular and Solid-State Behavior. Journal of the American Chemical Society, 2017, 139, 18456-18459.	6.6	87
6	Energy decomposition analysis of single bonds within Kohnâ€“Sham density functional theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12649-12656.	3.3	85
7	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. Journal of Chemical Theory and Computation, 2020, 16, 2340-2354.	2.3	85
8	Variational Energy Decomposition Analysis of Chemical Bonding. 1. Spin-Pure Analysis of Single Bonds. Journal of Chemical Theory and Computation, 2016, 12, 4812-4820.	2.3	56
9	From Intermolecular Interaction Energies and Observable Shifts to Component Contributions and Back Again: A Tale of Variational Energy Decomposition Analysis. Annual Review of Physical Chemistry, 2021, 72, 641-666.	4.8	55
10	Aryl Group Transfer from Tetraarylborato Anions to an Electrophilic Dicopper(I) Center and Mixed-Valence Î¼-Aryl Dicopper(I,II) Complexes. Journal of the American Chemical Society, 2016, 138, 6484-6491.	6.6	54
11	Synthetic control and empirical prediction of redox potentials for Co₄O₄ cubanes over a 1.4 V range: implications for catalyst design and evaluation of high-valent intermediates in water oxidation. Chemical Science, 2017, 8, 4274-4284.	3.7	50
12	Manganeseâ€“Cobalt Oxido Cubanes Relevant to Manganese-Doped Water Oxidation Catalysts. Journal of the American Chemical Society, 2017, 139, 5579-5587.	6.6	47
13	Isomer-specific vibronic structure of the 9-, 1-, and 2-anthracenyl radicals via slow photoelectron velocity-map imaging. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1698-1705.	3.3	44
14	Evidence for the Existence of Group 3 Terminal Methylidene Complexes. Organometallics, 2017, 36, 80-88.	1.1	43
15	Câ€“H Bond Activations by Monoanionic, PNP-Supported Scandium Dialkyl Complexes. Organometallics, 2015, 34, 4647-4655.	1.1	42
16	What Levels of Coupled Cluster Theory Are Appropriate for Transition Metal Systems? A Study Using Near-Exact Quantum Chemical Values for 3d Transition Metal Binary Compounds. Journal of Chemical Theory and Computation, 2019, 15, 5370-5385.	2.3	42
17	Biaryl Reductive Elimination Is Dramatically Accelerated by Remote Lewis Acid Binding to a 2,2â€²-Bipyrimidylâ€“Platinum Complex: Evidence for a Bidentate Ligand Dissociation Mechanism. Organometallics, 2016, 35, 1064-1069.	1.1	34
18	Clarifying the quantum mechanical origin of the covalent chemical bond. Nature Communications, 2020, 11, 4893.	5.8	34

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19	Silver nanoparticles supported on passivated silica: preparation and catalytic performance in alkyne semi-hydrogenation. Dalton Transactions, 2014, 43, 15138-15142.	1.6	31
20	Lewis acidâ€“base interactions between platinum(<scp>ii</scp>) diaryl complexes and bis(perfluorophenyl)zinc: strongly accelerated reductive elimination induced by a Z-type ligand. Chemical Communications, 2016, 52, 7039-7042.	2.2	28
21	Efficient and selective catalysis for hydrogenation and hydrosilation of alkenes and alkynes with PNP complexes of scandium and yttrium. Chemical Communications, 2017, 53, 11881-11884.	2.2	27
22	Quantifying the Role of Orbital Contraction in Chemical Bonding. Journal of Physical Chemistry Letters, 2017, 8, 1967-1972.	2.1	20
23	Monomeric, Divalent Vanadium Bis(arylamido) Complexes: Linkage Isomerism and Reactivity. Organometallics, 2019, 38, 1648-1663.	1.1	20
24	Vibrational and Electronic Structure of the Î±- and Î²-Naphthyl Radicals via Slow Photoelectron Velocity-Map Imaging. Journal of the American Chemical Society, 2015, 137, 1420-1423.	6.6	19
25	Dicopper Alkyl Complexes: Synthesis, Structure, and Unexpected Persistence. Organometallics, 2018, 37, 2807-2823.	1.1	19
26	Probing radicalâ€“molecule interactions with a second generation energy decomposition analysis of DFT calculations using absolutely localized molecular orbitals. Physical Chemistry Chemical Physics, 2020, 22, 12867-12885.	1.3	17
27	Siloxyaluminate and Siloxygallate Complexes as Models for Framework and Partially Hydrolyzed Framework Sites in Zeolites and Zeotypes. Chemistry - A European Journal, 2021, 27, 307-315.	1.7	2
28	Pattern-free generation and quantumÂmechanical scoring of ring-chain tautomers. Journal of Computer-Aided Molecular Design, 2021, 35, 417-431.	1.3	2