

Daniel S Levine

List of Publications by Year in descending order

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28
papers

1,728
citations

331670

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501196

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docs citations

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citing authors

#	ARTICLE	IF	CITATIONS
1	Siloxyaluminate and Siloxygallate Complexes as Models for Framework and Partially Hydrolyzed Framework Sites in Zeolites and Zeotypes. <i>Chemistry - A European Journal</i> , 2021, 27, 307-315.	3.3	2
2	Pattern-free generation and quantum-mechanical scoring of ring-chain tautomers. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 417-431.	2.9	2
3	From Intermolecular Interaction Energies and Observable Shifts to Component Contributions and Back Again: A Tale of Variational Energy Decomposition Analysis. <i>Annual Review of Physical Chemistry</i> , 2021, 72, 641-666.	10.8	55
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	3.0	518
5	The Ground State Electronic Energy of Benzene. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8922-8929.	4.6	90
6	Probing radical-molecule interactions with a second generation energy decomposition analysis of DFT calculations using absolutely localized molecular orbitals. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12867-12885.	2.8	17
7	Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2139-2159.	5.3	90
8	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2340-2354.	5.3	85
9	Clarifying the quantum mechanical origin of the covalent chemical bond. <i>Nature Communications</i> , 2020, 11, 4893.	12.8	34
10	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. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5370-5385.	5.3	42
11	Monomeric, Divalent Vanadium Bis(arylamido) Complexes: Linkage Isomerism and Reactivity. <i>Organometallics</i> , 2019, 38, 1648-1663.	2.3	20
12	Dicopper Alkyl Complexes: Synthesis, Structure, and Unexpected Persistence. <i>Organometallics</i> , 2018, 37, 2807-2823.	2.3	19
13	Quantifying the Role of Orbital Contraction in Chemical Bonding. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1967-1972.	4.6	20
14	Synthetic control and empirical prediction of redox potentials for Co ₄ O ₄ cubanes over a 1.4 V range: implications for catalyst design and evaluation of high-valent intermediates in water oxidation. <i>Chemical Science</i> , 2017, 8, 4274-4284.	7.4	50
15	Manganese-Cobalt Oxido Cubanes Relevant to Manganese-Doped Water Oxidation Catalysts. <i>Journal of the American Chemical Society</i> , 2017, 139, 5579-5587.	13.7	47
16	Efficient and selective catalysis for hydrogenation and hydrosilation of alkenes and alkynes with PNP complexes of scandium and yttrium. <i>Chemical Communications</i> , 2017, 53, 11881-11884.	4.1	27
17	Expanded Helicenes: A General Synthetic Strategy and Remarkable Supramolecular and Solid-State Behavior. <i>Journal of the American Chemical Society</i> , 2017, 139, 18456-18459.	13.7	87
18	Energy decomposition analysis of single bonds within Kohn-Sham density functional theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 12649-12656.	7.1	85

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19	Evidence for the Existence of Group 3 Terminal Methylidene Complexes. <i>Organometallics</i> , 2017, 36, 80-88.	2.3	43
20	Lewis acid–base interactions between platinum(II) diaryl complexes and bis(perfluorophenyl)zinc: strongly accelerated reductive elimination induced by a Z-type ligand. <i>Chemical Communications</i> , 2016, 52, 7039-7042.	4.1	28
21	Aryl Group Transfer from Tetraarylborato Anions to an Electrophilic Dicopper(I) Center and Mixed-Valence 1/4-Aryl Dicopper(I,II) Complexes. <i>Journal of the American Chemical Society</i> , 2016, 138, 6484-6491.	13.7	54
22	Variational Energy Decomposition Analysis of Chemical Bonding. 1. Spin-Pure Analysis of Single Bonds. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4812-4820.	5.3	56
23	Isomer-specific vibronic structure of the 9-, 1-, and 2-anthracenyl radicals via slow photoelectron velocity-map imaging. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 1698-1705.	7.1	44
24	Biaryl Reductive Elimination Is Dramatically Accelerated by Remote Lewis Acid Binding to a 2,2'-Bipyrimidyl–Platinum Complex: Evidence for a Bidentate Ligand Dissociation Mechanism. <i>Organometallics</i> , 2016, 35, 1064-1069.	2.3	34
25	Vibrational and Electronic Structure of the 1±- and 1²-Naphthyl Radicals via Slow Photoelectron Velocity-Map Imaging. <i>Journal of the American Chemical Society</i> , 2015, 137, 1420-1423.	13.7	19
26	C–H Bond Activations by Monoanionic, PNP-Supported Scandium Dialkyl Complexes. <i>Organometallics</i> , 2015, 34, 4647-4655.	2.3	42
27	Silver nanoparticles supported on passivated silica: preparation and catalytic performance in alkyne semi-hydrogenation. <i>Dalton Transactions</i> , 2014, 43, 15138-15142.	3.3	31
28	Isolation of Pure Disubstituted <i>E</i> Olefins through Mo-Catalyzed <i>Z</i> -Selective Ethenolysis of Stereoisomeric Mixtures. <i>Journal of the American Chemical Society</i> , 2011, 133, 11512-11514.	13.7	87