

A Daniel Boese

List of Publications by Year in descending order

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52
papers

5,638
citations

279798

23
h-index

182427

51
g-index

52
all docs

52
docs citations

52
times ranked

5257
citing authors

#	ARTICLE	IF	CITATIONS
1	Development of density functionals for thermochemical kinetics. <i>Journal of Chemical Physics</i> , 2004, 121, 3405-3416.	3.0	1,380
2	A new parametrization of exchange–correlation generalized gradient approximation functionals. <i>Journal of Chemical Physics</i> , 2001, 114, 5497-5503.	3.0	659
3	New exchange-correlation density functionals: The role of the kinetic-energy density. <i>Journal of Chemical Physics</i> , 2002, 116, 9559-9569.	3.0	454
4	Report on the sixth blind test of organic crystal structure prediction methods. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 439-459.	1.1	445
5	W3 theory: Robust computational thermochemistry in the kJ/mol accuracy range. <i>Journal of Chemical Physics</i> , 2004, 120, 4129-4141.	3.0	434
6	New generalized gradient approximation functionals. <i>Journal of Chemical Physics</i> , 2000, 112, 1670-1678.	3.0	332
7	Predicting the binding energies of H-bonded complexes: A comparative DFT study. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3939-3947.	2.8	225
8	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 709-716.	2.5	223
9	The role of the basis set: Assessing density functional theory. <i>Journal of Chemical Physics</i> , 2003, 119, 3005-3014.	3.0	181
10	From ab initio quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia. <i>Journal of Chemical Physics</i> , 2003, 119, 5965-5980.	3.0	153
11	Vibrational Spectra of the Azabenzenes Revisited: Anharmonic Force Fields. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3085-3096.	2.5	151
12	Density Functional Theory and Hydrogen Bonds: Are We There Yet?. <i>ChemPhysChem</i> , 2015, 16, 978-985.	2.1	129
13	Basis Set Limit Coupled Cluster Study of H-Bonded Systems and Assessment of More Approximate Methods. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11122-11133.	2.5	87
14	Assessment of various density functionals and basis sets for the calculation of molecular anharmonic force fields. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 830-845.	2.0	67
15	Accurate adsorption energies of small molecules on oxide surfaces: CO on MgO(001). <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16481.	2.8	64
16	Anharmonic force fields and thermodynamic functions using density functional theory. <i>Molecular Physics</i> , 2005, 103, 863-876.	1.7	59
17	The infrared spectrum of Au ¹⁹⁹ TMCO ₂ . <i>Journal of Chemical Physics</i> , 2005, 122, 154301.	3.0	56
18	Unusual hydrogen bonding behavior in binary complexes of coinage metal anions with water. <i>Journal of Chemical Physics</i> , 2005, 123, 084307.	3.0	46

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19	Assessment of Coupled Cluster Theory and more Approximate Methods for Hydrogen Bonded Systems. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4403-4413.	5.3	41
20	Efficient CO ₂ Insertion and Reduction Catalyzed by a Terminal Zinc Hydride Complex. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 6906-6909.	13.8	39
21	Accurate ab initio computation of thermochemical data for C ₃ H _x species. <i>Chemical Physics</i> , 2008, 346, 56-68.	1.9	37
22	Effects of counterpoise correction and basis set extrapolation on the MP2 geometries of hydrogen bonded dimers of ammonia, water, and hydrogen fluoride. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1230-1238.	2.8	31
23	Revised values for the X23 benchmark set of molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24333-24344.	2.8	31
24	Basis set limit coupled-cluster studies of hydrogen-bonded systems. <i>Molecular Physics</i> , 2015, 113, 1618-1629.	1.7	24
25	Development of Embedded and Performance of Density Functional Methods for Molecular Crystals. <i>Journal of Physical Chemistry A</i> , 2018, 122, 708-713.	2.5	22
26	Accurate adsorption energies for small molecules on oxide surfaces: CH ₄ /MgO(001) and C ₂ H ₆ /MgO(001). <i>Journal of Computational Chemistry</i> , 2016, 37, 2374-2385.	3.3	20
27	Embedded and DFT Calculations on the Crystal Structures of Small Alkanes, Notably Propane. <i>Crystal Growth and Design</i> , 2017, 17, 1636-1646.	3.0	18
28	Adsorption of Nitrogen-Containing Compounds on the (100) $\hat{\pm}$ -Quartz Surface: Ab Initio Cluster Approach. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3023-3034.	3.1	17
29	Anharmonic force fields of perchloric acid, HClO ₄ , and perchloric anhydride, Cl ₂ O ₇ . An extreme case of inner polarization. <i>Journal of Molecular Structure</i> , 2006, 780-781, 310-316.	3.6	15
30	Tetrahydrothiophene and Tetrahydrofuran, Computational and X-ray Studies in the Crystalline Phase. <i>Crystal Growth and Design</i> , 2015, 15, 1073-1081.	3.0	15
31	Infrared spectra of O ₂ ⁺ (CO ₂) _n clusters (n=1-6): Asymmetric docking at the $\hat{\epsilon}^*$ orbital. <i>Journal of Chemical Physics</i> , 2005, 123, 074316.	3.0	14
32	Constructing simple yet accurate potentials for describing the solvation of HCl/water clusters in bulk helium and nanodroplets. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14550.	2.8	13
33	Ethyl Acetate: X-ray, Solvent and Computed Structures. <i>ChemPhysChem</i> , 2013, 14, 799-804.	2.1	13
34	Towards hybrid density functional calculations of molecular crystals via fragment-based methods. <i>Journal of Chemical Physics</i> , 2018, 149, 124104.	3.0	13
35	The hemibond as an alternative condensed phase structure for the hydroxyl radical. <i>Canadian Journal of Chemistry</i> , 2013, 91, 544-551.	1.1	12
36	CO Molecules on a NaCl(100) Surface: Structures, Energetics, and Vibrational Davydov Splittings at Various Coverages. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12637-12653.	3.1	12

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37	Interaction Between Gold Atoms and Thio-Aryl Ligands on the Au(111) Surface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 24871-24879.	3.1	11
38	Efficient CO ₂ Insertion and Reduction Catalyzed by a Terminal Zinc Hydride Complex. <i>Angewandte Chemie</i> , 2018, 130, 7022-7025.	2.0	11
39	ZMP-SAPT: DFT-SAPT using <i>ab initio</i> densities. <i>Journal of Chemical Physics</i> , 2019, 150, 154101.	3.0	10
40	Rozen's Epoxidation Reagent, CH ₃ CNÂ•HOF: A Theoretical Study of Its Structure, Vibrational Spectroscopy, and Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8275-8281.	2.5	9
41	Mechanism of O(³ P) Formation from a Hydroxyl Radical Pair in Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4740-4748.	5.3	9
42	Cross-talk between amino acid residues and flavonoid derivatives: insights into their chemical recognition. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15682.	2.8	8
43	Synthesis and Characterization of a Thiopyridazinylmethane-Based Scorpionate Ligand: Formation of Zinc Complexes and Rearrangement Reaction. <i>Organometallics</i> , 2017, 36, 3790-3798.	2.3	8
44	Electron-rich triarylphosphines as nucleophilic catalysts for oxa-Michael reactions. <i>Beilstein Journal of Organic Chemistry</i> , 2021, 17, 1689-1697.	2.2	8
45	Water as a monomer: synthesis of an aliphatic polyethersulfone from divinyl sulfone and water. <i>Chemical Science</i> , 2022, 13, 6920-6928.	7.4	8
46	MMH-2 as a new approach for the prediction of intermolecular interactions: the crystal packing of acetamide. <i>CrystEngComm</i> , 2009, 11, 2358.	2.6	7
47	Adjusting dispersion parameters for the density-functional tight-binding description of molecular crystals. <i>Chemical Physics Letters</i> , 2019, 718, 7-11.	2.6	5
48	On the Regioselectivity of the Gould-Jacobs Reaction: Gas-Phase Versus Solution-Phase Thermolysis. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 7051-7061.	2.4	5
49	Non-Planar Structures of Sterically Overcrowded Trialkylamines. <i>Chemistry - A European Journal</i> , 2021, 27, 3700-3707.	3.3	3
50	Addendum: Assessment of Coupled Cluster Theory and more Approximate Methods for Hydrogen Bonded Systems. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 893-893.	5.3	2
51	Intramolecular resonance-assisted hydrogen bonds: Insights from symmetry adapted perturbation theory. <i>Chemical Physics</i> , 2022, 557, 111474.	1.9	2
52	Adsorption of nitrogen-containing compounds on hydroxylated α -quartz surfaces. <i>RSC Advances</i> , 2019, 9, 36066-36074.	3.6	0