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	Intramolecular resonance-assisted hydrogen bonds: Insights from symmetry adapted perturbation theory. Chemical Physics, 2022, 557, 111474.	1.9	2
2	Water as a monomer: synthesis of an aliphatic polyethersulfone from divinyl sulfone and water. Chemical Science, 2022, 13, 6920-6928.	7.4	8
3	Nonâ€Planar Structures of Sterically Overcrowded Trialkylamines. Chemistry - A European Journal, 2021, 27, 3700-3707.	3.3	3
4	Electron-rich triarylphosphines as nucleophilic catalysts for oxa-Michael reactions. Beilstein Journal of Organic Chemistry, 2021, 17, 1689-1697.	2.2	8
5	On the Regioselectivity of the Gouldâ€“Jacobs Reaction: Gasâ€Phase Versus Solutionâ€Phase Thermolysis. European Journal of Organic Chemistry, 2020, 2020, 7051-7061.	2.4	5
6	Adjusting dispersion parameters for the density-functional tight-binding description of molecular crystals. Chemical Physics Letters, 2019, 718, 7-11.	2.6	5
7	ZMP-SAPT: DFT-SAPT using ab initio densities. Journal of Chemical Physics, 2019, 150, 154101.	3.0	10
8	Revised values for the X23 benchmark set of molecular crystals. Physical Chemistry Chemical Physics, 2019, 21, 24333-24344.	2.8	31
9	Adsorption of nitrogen-containing compounds on hydroxylated Î±-quartz surfaces. RSC Advances, 2019, 9, 36066-36074.	3.6	0
10	Efficient CO₂ Insertion and Reduction Catalyzed by a Terminal Zinc Hydride Complex. Angewandte Chemie, 2018, 130, 7022-7025.	2.0	11
11	Efficient CO₂ Insertion and Reduction Catalyzed by a Terminal Zinc Hydride Complex. Angewandte Chemie - International Edition, 2018, 57, 6906-6909.	13.8	39
12	Development of Embedded and Performance of Density Functional Methods for Molecular Crystals. Journal of Physical Chemistry A, 2018, 122, 708-713.	2.5	22
13	Towards hybrid density functional calculations of molecular crystals via fragment-based methods. Journal of Chemical Physics, 2018, 149, 124104.	3.0	13
14	Embedded and DFT Calculations on the Crystal Structures of Small Alkanes, Notably Propane. Crystal Growth and Design, 2017, 17, 1636-1646.	3.0	18
15	Synthesis and Characterization of a Thiopyridazinylmethane-Based Scorpionate Ligand: Formation of Zinc Complexes and Rearrangement Reaction. Organometallics, 2017, 36, 3790-3798.	2.3	8
16	CO Molecules on a NaCl(100) Surface: Structures, Energetics, and Vibrational Davydov Splittings at Various Coverages. Journal of Physical Chemistry C, 2016, 120, 12637-12653.	3.1	12
17	Accurate adsorption energies for small molecules on oxide surfaces: CH₄/MgO(001) and C₂H₆/MgO(001). Journal of Computational Chemistry, 2016, 37, 2374-2385.	3.3	20
18	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445

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19	Tetrahydrothiophene and Tetrahydrofuran, Computational and X-ray Studies in the Crystalline Phase. Crystal Growth and Design, 2015, 15, 1073-1081.	3.0	15
20	Density Functional Theory and Hydrogen Bonds: Are We There Yet?. ChemPhysChem, 2015, 16, 978-985.	2.1	129
21	Basis set limit coupled-cluster studies of hydrogen-bonded systems. Molecular Physics, 2015, 113, 1618-1629.	1.7	24
22	Mechanism of O(³P) Formation from a Hydroxyl Radical Pair in Aqueous Solution. Journal of Chemical Theory and Computation, 2015, 11, 4740-4748.	5.3	9
23	Adsorption of Nitrogen-Containing Compounds on the (100) Î±-Quartz Surface: Ab Initio Cluster Approach. Journal of Physical Chemistry C, 2014, 118, 3023-3034.	3.1	17
24	Addendum: Assessment of Coupled Cluster Theory and more Approximate Methods for Hydrogen Bonded Systems. Journal of Chemical Theory and Computation, 2014, 10, 893-893.	5.3	2
25	Accurate adsorption energies of small molecules on oxide surfaces: COâ€“MgO(001). Physical Chemistry Chemical Physics, 2013, 15, 16481.	2.8	64
26	Assessment of Coupled Cluster Theory and more Approximate Methods for Hydrogen Bonded Systems. Journal of Chemical Theory and Computation, 2013, 9, 4403-4413.	5.3	41
27	The hemibond as an alternative condensed phase structure for the hydroxyl radical. Canadian Journal of Chemistry, 2013, 91, 544-551.	1.1	12
28	Ethyl Acetate: Xâ€ray, Solvent and Computed Structures. ChemPhysChem, 2013, 14, 799-804.	2.1	13
29	Cross-talk between amino acid residues and flavonoid derivatives: insights into their chemical recognition. Physical Chemistry Chemical Physics, 2012, 14, 15682.	2.8	8
30	Constructing simple yet accurate potentials for describing the solvation of HCl/waterclusters in bulk helium and nanodroplets. Physical Chemistry Chemical Physics, 2011, 13, 14550.	2.8	13
31	Interaction Between Gold Atoms and Thio-Aryl Ligands on the Au(111) Surface. Journal of Physical Chemistry C, 2011, 115, 24871-24879.	3.1	11
32	Effects of counterpoise correction and basis set extrapolation on the MP2 geometries of hydrogen bonded dimers of ammonia, water, and hydrogen fluoride. Physical Chemistry Chemical Physics, 2011, 13, 1230-1238.	2.8	31
33	MMH-2 as a new approach for the prediction of intermolecular interactions: the crystal packing of acetamide. CrystEngComm, 2009, 11, 2358.	2.6	7
34	Accurate ab initio computation of thermochemical data for C3Hx species. Chemical Physics, 2008, 346, 56-68.	1.9	37
35	Basis Set Limit Coupled Cluster Study of H-Bonded Systems and Assessment of More Approximate Methods. Journal of Physical Chemistry A, 2007, 111, 11122-11133.	2.5	87
36	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactionsâ€. Journal of Physical Chemistry A, 2006, 110, 709-716.	2.5	223

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37	Rozen's Epoxidation Reagent, CH3CNÂ·HOF:Â A Theoretical Study of Its Structure, Vibrational Spectroscopy, and Reaction Mechanismâ€. Journal of Physical Chemistry A, 2006, 110, 8275-8281.	2.5	9
38	Anharmonic force fields of perchloric acid, HClO4, and perchloric anhydride, Cl2O7. An extreme case of inner polarization. Journal of Molecular Structure, 2006, 780-781, 310-316.	3.6	15
39	Assessment of various density functionals and basis sets for the calculation of molecular anharmonic force fields. International Journal of Quantum Chemistry, 2005, 104, 830-845.	2.0	67
40	Unusual hydrogen bonding behavior in binary complexes of coinage metal anions with water. Journal of Chemical Physics, 2005, 123, 084307.	3.0	46
41	Infrared spectra of O2â^'â^™(CO2)n clusters (n=1â€“6): Asymmetric docking at the Ï€* orbital. Journal of Chemical Physics, 2005, 123, 074316.	3.0	14
42	The infrared spectrum of Auâ^'â^™CO2. Journal of Chemical Physics, 2005, 122, 154301.	3.0	56
43	Anharmonic force fields and thermodynamic functions using density functional theory. Molecular Physics, 2005, 103, 863-876.	1.7	59
44	W3 theory: Robust computational thermochemistry in the kJ/mol accuracy range. Journal of Chemical Physics, 2004, 120, 4129-4141.	3.0	434
45	Vibrational Spectra of the Azabenzenes Revisited:Â Anharmonic Force Fieldsâ€. Journal of Physical Chemistry A, 2004, 108, 3085-3096.	2.5	151
46	Development of density functionals for thermochemical kinetics. Journal of Chemical Physics, 2004, 121, 3405-3416.	3.0	1,380
47	The role of the basis set: Assessing density functional theory. Journal of Chemical Physics, 2003, 119, 3005-3014.	3.0	181
48	From ab initio quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia. Journal of Chemical Physics, 2003, 119, 5965-5980.	3.0	153
49	New exchange-correlation density functionals: The role of the kinetic-energy density. Journal of Chemical Physics, 2002, 116, 9559-9569.	3.0	454
50	A new parametrization of exchangeâ€“correlation generalized gradient approximation functionals. Journal of Chemical Physics, 2001, 114, 5497-5503.	3.0	659
51	New generalized gradient approximation functionals. Journal of Chemical Physics, 2000, 112, 1670-1678.	3.0	332
52	Predicting the binding energies of H-bonded complexes: A comparative DFT study. Physical Chemistry Chemical Physics, 1999, 1, 3939-3947.	2.8	225