Adrian Daniel Boese

List of Publications by Year
in descending order

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66 papers	5,995 citations	201674 27 h-index	106344 65 g-index
70 all docs	70 docs citations	70 times ranked	5797 citing authors

#	Article	IF	Citations
1	Development of density functionals for thermochemical kinetics. Journal of Chemical Physics, 2004, 121, 3405-3416.	3.0	1,380
2	A new parametrization of exchangeâ€“correlation generalized gradient approximation functionals. Journal of Chemical Physics, 2001, 114, 5497-5503.	3.0	659
3	New exchange-correlation density functionals: The role of the kinetic-energy density. Journal of Chemical Physics, 2002, 116, 9559-9569.	3.0	454
4	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
5	W3 theory: Robust computational thermochemistry in the kJ/mol accuracy range. Journal of Chemical Physics, 2004, 120, 4129-4141.	3.0	434
6	New generalized gradient approximation functionals. Journal of Chemical Physics, 2000, 112, 1670-1678.	3.0	332
7	Predicting the binding energies of H-bonded complexes: A comparative DFT study. Physical Chemistry Chemical Physics, 1999, 1, 3939-3947.	2.8	225
8	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactionsâ€. Journal of Physical Chemistry A, 2006, 110, 709-716.	2.5	223
9	The role of the basis set: Assessing density functional theory. Journal of Chemical Physics, 2003, 119, 3005-3014.	3.0	181
10	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
11	Vibrational Spectra of the Azabenzenes Revisited:Â Anharmonic Force Fieldsâ€. Journal of Physical Chemistry A, 2004, 108, 3085-3096.	2.5	151
12	Density Functional Theory and Hydrogen Bonds: Are We There Yet?. ChemPhysChem, 2015, 16, 978-985.	2.1	129
13	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
14	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
15	C2 fragmentation energy of C60 revisited: theory disagrees with most experiments. Chemical Physics Letters, 1998, 294, 233-236.	2.6	64
16	Accurate adsorption energies of small molecules on oxide surfaces: COâ€“MgO(001). Physical Chemistry Chemical Physics, 2013, 15, 16481.	2.8	64
17	How to control single-molecule rotation. Nature Communications, 2019, 10, 4631.	12.8	61
18	Anharmonic force fields and thermodynamic functions using density functional theory. Molecular Physics, 2005, 103, 863-876.	1.7	59

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19	The infrared spectrum of Auâ^'â^™CO2. Journal of Chemical Physics, 2005, 122, 154301.	3.0	56
20	The Surprising Crystal Packing of Chlorinefluoride. Angewandte Chemie International Edition in English, 1997, 36, 1489-1492.	4.4	54
21	Ab Initio Study of the Adsorption of Small Molecules on Metalâ€"Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion. Inorganic Chemistry, 2015, 54, 8251-8263.	4.0	48
22	Unusual hydrogen bonding behavior in binary complexes of coinage metal anions with water. Journal of Chemical Physics, 2005, 123, 084307.	3.0	46
23	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
24	Efficient CO₂ Insertion and Reduction Catalyzed by a Terminal Zinc Hydride Complex. Angewandte Chemie - International Edition, 2018, 57, 6906-6909.	13.8	39
25	Energy Ordering of Molecular Orbitals. Journal of Physical Chemistry Letters, 2017, 8, 208-213.	4.6	38
26	Accurate ab initio computation of thermochemical data for C3Hx species. Chemical Physics, 2008, 346, 56-68.	1.9	37
27	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
28	Revised values for the X23 benchmark set of molecular crystals. Physical Chemistry Chemical Physics, 2019, 21, 24333-24344.	2.8	31
29	Basis set limit coupled-cluster studies of hydrogen-bonded systems. Molecular Physics, 2015, 113, 1618-1629.	1.7	24
30	Development of Embedded and Performance of Density Functional Methods for Molecular Crystals. Journal of Physical Chemistry A, 2018, 122, 708-713.	2.5	22
31	Strontium-free rare earth perovskite ferrites with fast oxygen exchange kinetics: Experiment and theory. Journal of Solid State Chemistry, 2018, 259, 57-66.	2.9	21
32	The vibrational spectrum of FeO2+ isomersâ€"Theoretical benchmark and experiment. Journal of Chemical Physics, 2014, 140, 204315.	3.0	20
33	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
34	AB INITIO MOLECULAR DYNAMICS STUDY OF DISSOLVED SiO2 IN SUPERCRITICAL WATER. Journal of Theoretical and Computational Chemistry, 2007, 06, 49-62.	1.8	18
35	Embedded and DFT Calculations on the Crystal Structures of Small Alkanes, Notably Propane. Crystal Growth and Design, 2017, 17, 1636-1646.	3.0	18
36	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

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37	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
38	Tetrahydrothiophene and Tetrahydrofuran, Computational and X-ray Studies in the Crystalline Phase. Crystal Growth and Design, 2015, 15, 1073-1081.	3.0	15
39	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
40	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
41	Ethyl Acetate: Xâ€ray, Solvent and Computed Structures. ChemPhysChem, 2013, 14, 799-804.	2.1	13
42	Towards hybrid density functional calculations of molecular crystals via fragment-based methods. Journal of Chemical Physics, 2018, 149, 124104.	3.0	13
43	The hemibond as an alternative condensed phase structure for the hydroxyl radical. Canadian Journal of Chemistry, 2013, 91, 544-551.	1.1	12
44	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
45	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
46	Efficient CO₂ Insertion and Reduction Catalyzed by a Terminal Zinc Hydride Complex. Angewandte Chemie, 2018, 130, 7022-7025.	2.0	11
47	Infrared multiphoton electron detachment spectroscopy of C762â^'. Journal of Chemical Physics, 2009, 131, 124306.	3.0	10
48	ZMP-SAPT: DFT-SAPT using ab initio densities. Journal of Chemical Physics, 2019, 150, 154101.	3.0	10
49	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
50	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
51	Die Ã¼berraschende Kristallpackung von Chlorfluorid. Angewandte Chemie, 1997, 109, 1538-1541.	2.0	8
52	Cross-talk between amino acid residues and flavonoid derivatives: insights into their chemical recognition. Physical Chemistry Chemical Physics, 2012, 14, 15682.	2.8	8
53	Synthesis and Characterization of a Thiopyridazinylmethane-Based Scorpionate Ligand: Formation of Zinc Complexes and Rearrangement Reaction. Organometallics, 2017, 36, 3790-3798.	2.3	8
54	Electron-rich triarylphosphines as nucleophilic catalysts for oxa-Michael reactions. Beilstein Journal of Organic Chemistry, 2021, 17, 1689-1697.	2.2	8

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55	Water as a monomer: synthesis of an aliphatic polyethersulfone from divinyl sulfone and water. Chemical Science, 2022, 13, 6920-6928.	7.4	8
56	MMH-2 as a new approach for the prediction of intermolecular interactions: the crystal packing of acetamide. CrystEngComm, 2009, 11, 2358.	2.6	7
57	Catalytic reduction of nitrate by an oxidorhenium (V) complex. Journal of Catalysis, 2021, 397, 108-115.	6.2	6
58	Adjusting dispersion parameters for the density-functional tight-binding description of molecular crystals. Chemical Physics Letters, 2019, 718, 7-11.	2.6	5
59	Mechanistic Studies of the TRIP-Catalyzed Allylation with Organozinc Reagents. Journal of Organic Chemistry, 2020, 85, 9672-9679.	3.2	5
60	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
61	The Protonation Site of Aniline Revisited: A 'Torture Test' for Electron Correlation Methods. ACS Symposium Series, 2007, , 183-192.	0.5	3
62	Nonâ€Planar Structures of Sterically Overcrowded Trialkylamines. Chemistry - A European Journal, 2021, 27, 3700-3707.	3.3	3
63	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
64	Intramolecular resonance-assisted hydrogen bonds: Insights from symmetry adapted perturbation theory. Chemical Physics, 2022, 557, 111474.	1.9	2
65	Cold inelastic collisions of He(¹S) with the smallest astrophysical anion observed, CN^{â^'}(¹Î£⁺): an accurate quantum dynamical study.. Journal of Physics: Conference Series, 2017, 875, 102018.	0.4	1
66	Adsorption of nitrogen-containing compounds on hydroxylated Î±-quartz surfaces. RSC Advances, 2019, 9, 36066-36074.	3.6	0