Tore Brinck

List of Publications by Year in descending order

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142	9,289	41344	42399
papers	citations	49 h-index	92 g-index

160	160	160	7751
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantitative analysis of molecular surfaces: areas, volumes, electrostatic potentials and average local ionization energies. Journal of Molecular Modeling, 2010, 16, 1679-1691.	1.8	985
2	Tuning the HOMO and LUMO Energy Levels of Organic Chromophores for Dye Sensitized Solar Cells. Journal of Organic Chemistry, 2007, 72, 9550-9556.	3.2	576
3	Surface electrostatic potentials of halogenated methanes as indicators of directional intermolecular interactions. International Journal of Quantum Chemistry, 1992, 44, 57-64.	2.0	370
4	Average local ionization energies on the molecular surfaces of aromatic systems as guides to chemical reactivity. Canadian Journal of Chemistry, 1990, 68, 1440-1443.	1.1	363
5	Carbonâ^'Carbon Bonds by Hydrolytic Enzymes. Journal of the American Chemical Society, 2003, 125, 874-875.	13.7	249
6	Mechanism of H₂O₂ Decomposition on Transition Metal Oxide Surfaces. Journal of Physical Chemistry C, 2012, 116, 9533-9543.	3.1	223
7	Polarizability and volume. Journal of Chemical Physics, 1993, 98, 4305-4306.	3.0	216
8	HCCI experiments with toluene reference fuels modeled by a semidetailed chemical kinetic model. Combustion and Flame, 2008, 155, 696-712.	5.2	195
9	Statistically-based interaction indices derived from molecular surface electrostatic potentials: a general interaction properties function (GIPF). Computational and Theoretical Chemistry, 1994, 307, 55-64.	1.5	183
10	Rhodaninedyes for dye-sensitized solar cellsâ€‰:â€‰ spectroscopy, energy levels and photovoltaic performance. Physical Chemistry Chemical Physics, 2009, 11, 133-141.	2.8	178
11	Symmetric and unsymmetric donor functionalization. comparing structural and spectral benefits of chromophores for dye-sensitized solar cells. Journal of Materials Chemistry, 2009, 19, 7232.	6.7	177
12	Synthesis and Mechanistic Studies of Organic Chromophores with Different Energy Levels for p-Type Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2010, 114, 4738-4748.	3.1	174
13	High Incident Photonâ€toâ€Current Conversion Efficiency of pâ€Type Dyeâ€Sensitized Solar Cells Based on NiO and Organic Chromophores. Advanced Materials, 2009, 21, 2993-2996.	21.0	173
14	A Computational Analysis of Substituent Effects on the Oâ^'H Bond Dissociation Energy in Phenols:Â Polar Versus Radical Effects. Journal of the American Chemical Society, 1997, 119, 4239-4244.	13.7	170
15	Family-independent relationships between computed molecular surface quantities and solute hydrogen bond acidity/basicity and solute-induced methanol Oâ€“H infrared frequency shifts. Canadian Journal of Chemistry, 1995, 73, 483-488.	1.1	164
16	Molecular surface electrostatic potentials and local ionization energies of Group V-VII hydrides and their anions: Relationships for aqueous and gas-phase acidities. International Journal of Quantum Chemistry, 1993, 48, 73-88.	2.0	146
17	Extending the Ïƒ-Hole Concept to Metals: An Electrostatic Interpretation of the Effects of Nanostructure in Gold and Platinum Catalysis. Journal of the American Chemical Society, 2017, 139, 11012-11015.	13.7	136
18	Exploring the Active-Site of a Rationally Redesigned Lipase for Catalysis of Michael-Type Additions. ChemBioChem, 2005, 6, 331-336.	2.6	135

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19	Quantitative determination of the total local polarity (charge separation) in molecules. Molecular Physics, 1992, 76, 609-617.	1.7	118
20	Correlations between molecular electrostatic potentials and some experimentally-based indices of reactivity. Computational and Theoretical Chemistry, 1992, 256, 29-45.	1.5	114
21	Detection of pentazolate anion (cyclo-N5â¯) from laser ionization and decomposition of solid p-dimethylaminophenylpentazole. Chemical Physics Letters, 2003, 379, 539-546.	2.6	114
22	Machine learning meets mechanistic modelling for accurate prediction of experimental activation energies. Chemical Science, 2021, 12, 1163-1175.	7.4	102
23	Theoretical Studies of the Hydrolysis of the Methyl Phosphate Anion. Journal of Physical Chemistry A, 1999, 103, 5379-5386.	2.5	100
24	Ïƒ-Holes and Ïƒ-lumps direct the Lewis basic and acidic interactions of noble metal nanoparticles: introducing regium bonds. Physical Chemistry Chemical Physics, 2018, 20, 2676-2692.	2.8	99
25	Prediction of Solubility of Solid Organic Compounds in Solvents by UNIFAC. Industrial & Engineering Chemistry Research, 2002, 41, 5114-5124.	3.7	98
26	A computational analysis of the bonding in boron trifluoride and boron trichloride and their complexes with ammonia. Inorganic Chemistry, 1993, 32, 2622-2625.	4.0	94
27	Radial behavior of the average local ionization energies of atoms. Journal of Chemical Physics, 1991, 95, 6699-6704.	3.0	88
28	Relationships of molecular surface electrostatic potentials to some macroscopic properties. Chemical Physics, 1996, 204, 289-299.	1.9	85
29	Phosphine-catalyzed disulfide metathesis. Chemical Communications, 2008, , 6603.	4.1	85
30	Relationships of critical constants and boiling points to computed molecular surface properties. The Journal of Physical Chemistry, 1993, 97, 9369-9373.	2.9	81
31	Direct Epoxidation in Candida antarctica Lipase B Studied by Experiment and Theory. ChemBioChem, 2008, 9, 2443-2451.	2.6	78
32	On the method-dependence of transition state asynchronicity in Dielsâ€“Alder reactions. Physical Chemistry Chemical Physics, 2013, 15, 5108.	2.8	76
33	Relationships between the aqueous acidities of some carbon, oxygen, and nitrogen acids and the calculated surface local ionization energies of their conjugate bases. Journal of Organic Chemistry, 1991, 56, 5012-5015.	3.2	74
34	Thiol-ene coupling reaction of fatty acid monomers. Journal of Polymer Science Part A, 2004, 42, 6346-6352.	2.3	74
35	Reactivity of metal oxide clusters with hydrogen peroxide and water â€“ a DFT study evaluating the performance of different exchangeâ€“correlation functionals. Physical Chemistry Chemical Physics, 2013, 15, 5539.	2.8	73
36	Octanol/water partition coefficients expressed in terms of solute molecular surface areas and electrostatic potentials. Journal of Organic Chemistry, 1993, 58, 7070-7073.	3.2	69

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37	Kinetic Stability and Propellant Performance of Green Energetic Materials. Chemistry - A European Journal, 2010, 16, 6590-6600.	3.3	69
38	A relationship between experimentally determined pKas and molecular surface ionization energies for some azines and azoles. Journal of Organic Chemistry, 1991, 56, 2934-2936.	3.2	68
39	Calculated electrostatic potentials and local surface ionization energies of para-substituted anilines as measures of substituent effects. Canadian Journal of Chemistry, 1992, 70, 2209-2214.	1.1	66
40	Quantum Chemical Studies on the Thermochemistry of Alkyl and Peroxyl Radicals. Journal of Physical Chemistry A, 1999, 103, 7094-7104.	2.5	65
41	Aldol additions with mutant lipase: analysis by experiments and theoretical calculations. Journal of Molecular Catalysis B: Enzymatic, 2004, 31, 123-128.	1.8	65
42	Investigation of relationships between solute molecule surface electrostatic potentials and solubilities in supercritical fluids. The Journal of Physical Chemistry, 1992, 96, 7938-7943.	2.9	62
43	Applications of calculated local surface ionization energies to chemical reactivity. Computational and Theoretical Chemistry, 1992, 255, 271-281.	1.5	62
44	The Stability of Arylpentazoles. Journal of Physical Chemistry A, 2004, 108, 7463-7467.	2.5	58
45	Ab initio and density functional theory studies of the catalytic mechanism for ester hydrolysis in serine hydrolases. International Journal of Quantum Chemistry, 1998, 69, 89-103.	2.0	54
46	Molecular dynamics study of zinc binding to cysteines in a peptide mimic of the alcohol dehydrogenase structural zinc site. Physical Chemistry Chemical Physics, 2009, 11, 975-983.	2.8	54
47	A Theoretical Study of the Uncatalyzed and BF3-Assisted Baeyerâ^'Villiger Reactions. Journal of Organic Chemistry, 2001, 66, 1193-1199.	3.2	53
48	Stepwise Dielsâ€“Alder: More than Just an Oddity? A Computational Mechanistic Study. Journal of Organic Chemistry, 2012, 77, 6563-6573.	3.2	52
49	A theoretical study of the azide (N3) doublet states. A new route to tetraazatetrahedrane (N4): N+N3â†'N4. Journal of Chemical Physics, 2002, 116, 9740-9748.	3.0	50
50	Electrostatic potentials on the molecular surfaces of cyclic ureides. The Journal of Physical Chemistry, 1991, 95, 844-848.	2.9	49
51	Relationships between solute molecular properties and solubility in supercritical carbon dioxide. The Journal of Physical Chemistry, 1993, 97, 729-732.	2.9	48
52	The Surface Structure of Cu₂O(100). Journal of Physical Chemistry C, 2016, 120, 4373-4381.	3.1	46
53	Theoretical Study of the Triplet N4Potential Energy Surface. Journal of Physical Chemistry A, 2000, 104, 11999-12005.	2.5	45
54	Prediction of waterâ€“octanol partition coefficients using theoretical descriptors derived from the molecular surface area and the electrostatic potential. Journal of the Chemical Society Perkin Transactions II, 1997, , 289-294.	0.9	42

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55	Validation of a Computational Model for Predicting the Site for Electrophilic Substitution in Aromatic Systems. Journal of Organic Chemistry, 2010, 75, 4696-4705.	3.2	42
56	Electrostatics and polarization determine the strength of the halogen bond: a red card for charge transfer. Journal of Molecular Modeling, 2019, 25, 125.	1.8	42
57	Relationships between computed molecular properties and solute-solvent interactions in supercritical solutions. The Journal of Physical Chemistry, 1993, 97, 5144-5148.	2.9	38
58	Diastereoselective One-Pot Tandem Synthesis of 3-Substituted Isoindolinones: A Mechanistic Investigation. Journal of Organic Chemistry, 2010, 75, 5882-5887.	3.2	38
59	Experimental Detection of Trinitramide, N(NO₂)₃. Angewandte Chemie - International Edition, 2011, 50, 1145-1148.	13.8	38
60	Nucleophilic Aromatic Substitution Reactions Described by the Local Electron Attachment Energy. Journal of Organic Chemistry, 2017, 82, 3072-3083.	3.2	38
61	The use of the electrostatic potential at the molecular surface in recognition interactions: Dibenzo-p-dioxinsand related systems. Journal of Molecular Graphics, 1990, 8, 81-85.	1.1	37
62	Racemase Activity of B. cepacia Lipase Leads to Dualâ€Function Asymmetric Dynamic Kinetic Resolution of Î±â€Aminonitriles. Angewandte Chemie - International Edition, 2011, 50, 6592-6595.	13.8	37
63	Predicting Regioselectivity in Nucleophilic Aromatic Substitution. Journal of Organic Chemistry, 2012, 77, 3262-3269.	3.2	37
64	On the Anomalous Decomposition and Reactivity of Ammonium and Potassium Dinitramide. Journal of Physical Chemistry A, 2010, 114, 2845-2854.	2.5	36
65	The Molecular Surface Property Approach: A Guide to Chemical Interactions in Chemistry, Medicine, and Material Science. Advanced Theory and Simulations, 2019, 2, 1800149.	2.8	36
66	The catalytic effect of water in basic hydrolysis of methyl acetate: a theoretical study. Computational and Theoretical Chemistry, 1999, 459, 85-93.	1.5	34
67	Rational design of a lipase to accommodate catalysis of Baeyer?Villiger oxidation with hydrogen peroxide. Journal of Molecular Modeling, 2003, 9, 164-171.	1.8	34
68	Polymer-assisted laser desorption/ionization analysis of small molecular weight compounds. Rapid Communications in Mass Spectrometry, 2004, 18, 841-852.	1.5	34
69	Control of the ambident reactivity of the nitrite ion. Organic and Biomolecular Chemistry, 2013, 11, 648-653.	2.8	33
70	Partition coefficients of nitroaromatics expressed in terms of their molecular surface areas and electrostatic potentials. The Journal of Physical Chemistry, 1993, 97, 13807-13809.	2.9	31
71	In situ confocal Raman micro-spectroscopy and electrochemical studies of mussel adhesive protein and ceria composite film on carbon steel in salt solutions. Electrochimica Acta, 2013, 107, 276-291.	5.2	31
72	Computational Analysis of Substituent Effects in Para-Substituted Phenoxide Ions. The Journal of Physical Chemistry, 1996, 100, 10116-10120.	2.9	30

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73	Mechanism and regioselectivity of electrophilic aromatic nitration in solution: the validity of the transition state approach. Journal of Molecular Modeling, 2018, 24, 15.	1.8	29
74	In situ investigations of Fe3+ induced complexation of adsorbed Mefp-1 protein film on iron substrate. Journal of Colloid and Interface Science, 2013, 404, 62-71.	9.4	28
75	Thermochemistry of Arylselanyl Radicals and the Pertinent Ions in Acetonitrile. Journal of the American Chemical Society, 2003, 125, 2148-2157.	13.7	27
76	pH-Dependent Mutarotation of 1-Thioaldoses in Water. Unexpected Behavior of (2S)-d-Aldopyranoses. Journal of Organic Chemistry, 2010, 75, 6115-6121.	3.2	27
77	Local Electron Attachment Energy and Its Use for Predicting Nucleophilic Reactions and Halogen Bonding. Journal of Physical Chemistry A, 2016, 120, 10023-10032.	2.5	27
78	Ab initio study of the ground state and the first excited state of the rectangular (D2h)N4 molecule. Chemical Physics Letters, 2001, 347, 220-228.	2.6	26
79	Supramolecular Control in Carbohydrate Epimerization: Discovery of a New Anion Hostâ"Guest System. Journal of the American Chemical Society, 2008, 130, 15270-15271.	13.7	26
80	Mechanistic Insights into the Stepwise Dielsâ€"Alder Reaction of 4,6-Dinitrobenzofuroxan. Organic Letters, 2012, 14, 118-121.	4.6	26
81	Surface local ionization energies and electrostatic potentials of the conjugate bases of a series of cyclic hydrocarbons in relation to their aqueous acidities. International Journal of Quantum Chemistry, 1991, 40, 91-98.	2.0	25
82	Reaction of Peroxyl Radicals with Ozone in Water. Journal of Physical Chemistry A, 2003, 107, 676-681.	2.5	25
83	Solvation of Carbanions in Organic Solvents:â€‰ A Test of the Polarizable Continuum Model. Journal of Physical Chemistry B, 2000, 104, 9887-9893.	2.6	24
84	On the formation of hydrogen gas on copper in anoxic water. Journal of Chemical Physics, 2011, 135, 084709.	3.0	24
85	Searching for the thermodynamic limit â€" a DFT study of the step-wise water oxidation of the bipyramidal Cu₇cluster. Physical Chemistry Chemical Physics, 2014, 16, 2452-2464.	2.8	24
86	Theoretical study of the singlet electronically excited states of N4. Chemical Physics Letters, 2001, 340, 597-603.	2.6	23
87	Solvation of Sulfur-Centered Cations and Anions in Acetonitrile. Journal of Physical Chemistry A, 2002, 106, 8827-8833.	2.5	23
88	Dehydrogenation of methanol on Cu2O(100) and (111). Journal of Chemical Physics, 2017, 146, 244702.	3.0	23
89	Elucidation of the Thermochemical Properties of Triphenyl- or Tributyl-Substituted Si-, Ge-, and Sn-Centered Radicals by Means of Electrochemical Approaches and Computations. Journal of the American Chemical Society, 2005, 127, 2677-2685.	13.7	22
90	Theoretical Investigation into Rate-Determining Factors in Electrophilic Aromatic Halogenation. Journal of Physical Chemistry A, 2018, 122, 3270-3279.	2.5	22

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91	The use of the electrostatic potential for analysis and prediction of intermolecular interactions. Theoretical and Computational Chemistry, 1998, , 51-93.	0.4	21
92	Reactivity at the Cu₂O(100):Cuâ€“H₂O interface: a combined DFT and PES study. Physical Chemistry Chemical Physics, 2016, 18, 30570-30584.	2.8	21
93	Segmental analysis of molecular surface electrostatic potentials: application to enzyme inhibition. Journal of Molecular Modeling, 2003, 9, 77-83.	1.8	20
94	Some Perspectives on Sensitivity to Initiation of Detonation. , 2014, , 45-62.		20
95	Force field parameterization of copper(I)-olefin systems from density functional calculations. Computational and Theoretical Chemistry, 1997, 397, 39-50.	1.5	19
96	Computational prediction of relative group polarizabilities. International Journal of Quantum Chemistry, 2003, 95, 632-637.	2.0	19
97	Utilizing the Ïƒ-complex stability for quantifying reactivity in nucleophilic substitution of aromatic fluorides. Beilstein Journal of Organic Chemistry, 2013, 9, 791-799.	2.2	19
98	Modified Interaction Properties Function for the Analysis and Prediction of Lewis Basicities. Journal of Physical Chemistry A, 1997, 101, 3408-3415.	2.5	18
99	A combined molecular dynamics simulation and quantum chemical study on the mechanism for activation of the OxyR transcription factor by hydrogen peroxide. Organic and Biomolecular Chemistry, 2006, 4, 3468-3478.	2.8	18
100	Synergistic activation of the Dielsâ€“Alder reaction by an organic catalyst and substituents: a computational study. Organic and Biomolecular Chemistry, 2009, 7, 1304.	2.8	18
101	A pragmatic procedure for predicting regioselectivity in nucleophilic substitution of aromatic fluorides. Tetrahedron Letters, 2011, 52, 3150-3153.	1.4	18
102	Electrochemical, atomic force microscopy and infrared reflection absorption spectroscopy studies of pre-formed mussel adhesive protein films on carbon steel for corrosion protection. Thin Solid Films, 2012, 520, 7136-7143.	1.8	18
103	Application of reactivity descriptors to the catalytic decomposition of hydrogen peroxide at oxide surfaces. Computational and Theoretical Chemistry, 2015, 1070, 108-116.	2.5	18
104	Dinitraminic acid (HDN) isomerization and self-decomposition revisited. Chemical Physics, 2008, 348, 53-60.	1.9	17
105	Novel 1,3-Dipolar Cycloadditions of Dinitraminic Acid:â€‰ Implications for the Chemical Stability of Ammonium Dinitramide. Journal of Physical Chemistry A, 2008, 112, 2456-2463.	2.5	17
106	Surface Reactions of H₂O₂, H₂, and O₂ in Aqueous Systems Containing ZrO₂. Journal of Physical Chemistry C, 2016, 120, 1609-1614.	3.1	16
107	Ïƒ-Holes on Transition Metal Nanoclusters and Their Influence on the Local Lewis Acidity. Crystals, 2017, 7, 222.	2.2	16
108	Electrostatic potential as a measure of gas phase carbocation stability. International Journal of Quantum Chemistry, 2006, 106, 2904-2909.	2.0	15

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109	Asymmetric Synthesis of Adjacent Triâ€•and Tetrasubstituted Carbon Stereocenters: Organocatalytic Aldol Reaction of an Hydantoin Surrogate with Azaarene 2â€Carbaldehydes. Chemistry - A European Journal, 2019, 25, 12431-12438.	3.3	15
110	Computational Study of the Amination of Halobenzenes and Phenylpentazole. A Viable Route to Isolate the Pentazolate Anion?. Journal of Organic Chemistry, 2004, 69, 3222-3225.	3.2	14
111	The anomalous solid state decomposition of ammonium dinitramide: a matter of surface polarization. Chemical Communications, 2009, , 2896.	4.1	14
112	Novel Approach for Identifying Key Residues in Enzymatic Reactions: Proton Abstraction in Ketosteroid Isomerase. Journal of Physical Chemistry B, 2014, 118, 13050-13058.	2.6	14
113	Local Lewis Acidity of (TiO₂)_n (n = 7â€“10) Nanoparticles Characterized by DFT-Based Descriptors: Tools for Catalyst Design. Journal of Physical Chemistry C, 2017, 121, 27483-27492.	3.1	14
114	Computational analysis of the early stage of cuprous oxide sulphidation: a top-down process. Corrosion Engineering Science and Technology, 2017, 52, 50-53.	1.4	13
115	The Surface Structure of Cu2O(100): Nature of Defects. Journal of Physical Chemistry C, 2019, 123, 7696-7704.	3.1	13
116	Interaction of Atomic Hydrogen with the Cu₂O(100) and (111) Surfaces. Journal of Physical Chemistry C, 2019, 123, 22172-22180.	3.1	13
117	Utilizing the Surface Electrostatic Potential to Predict the Interactions of Pt and Ni Nanoparticles with Lewis Acids and Basesâ€”Ïƒ-Lumps and Ïƒ-Holes Govern the Catalytic Activities. Journal of Physical Chemistry C, 2020, 124, 14696-14705.	3.1	13
118	Some proposed criteria for simulants in supercritical systems. Computational and Theoretical Chemistry, 1993, 281, 107-111.	1.5	12
119	Computational design of a lipase for catalysis of the Diels-Alder reaction. Journal of Molecular Modeling, 2011, 17, 833-849.	1.8	12
120	Envisioning an enzymatic Dielsâ€“Alder reaction by in situ acidâ€“base catalyzed diene generation. Chemical Communications, 2012, 48, 5665.	4.1	12
121	Computational design of a Dielsâ€“Alderase from a thermophilic esterase: the importance of dynamics. Journal of Computer-Aided Molecular Design, 2012, 26, 1079-1095.	2.9	12
122	Aqueous Solvation and Surface Oxidation of the Cu₇ Nanoparticle: Insights from Theoretical Modeling. Journal of Physical Chemistry C, 2016, 120, 1977-1988.	3.1	12
123	On the Kinetic and Thermodynamic Properties of Aryl Radicals Using Electrochemical and Theoretical Approaches. ChemElectroChem, 2017, 4, 3212-3221.	3.4	12
124	Designing a New Dielsâ€“Alderase: A Combinatorial, Semirational Approach Including Dynamic Optimization.. Journal of Chemical Information and Modeling, 2011, 51, 1906-1917.	5.4	11
125	Interaction of Sulfur Dioxide and Near-Ambient Pressures of Water Vapor with Cuprous Oxide Surfaces. Journal of Physical Chemistry C, 2017, 121, 24011-24024.	3.1	11
126	How Does Methyllithium Invert? A Density Functional Study. Organometallics, 2001, 20, 5134-5138.	2.3	10

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127	The local electron attachment energy and the electrostatic potential as descriptors of surfaceâ€“adsorbate interactions. Physical Chemistry Chemical Physics, 2019, 21, 17001-17009.	2.8	10
128	Ionization of ammonium dinitramide: decomposition pathways and ionization products. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	9
129	Dual Lewis Acid/Lewis Base Catalyzed Acylcyanation of Aldehydes: A Mechanistic Study. Chemistry - A European Journal, 2016, 22, 3821-3829.	3.3	9
130	The Molecular Surface Structure of Ammonium and Potassium Dinitramide: A Vibrational Sum Frequency Spectroscopy and Quantum Chemical Study. Journal of Physical Chemistry C, 2011, 115, 10588-10596.	3.1	7
131	Analytical Representation and Prediction of Macroscopic Properties. ACS Symposium Series, 1995, , 109-118.	0.5	6
132	Electronic structure calculations as a tool in the quest for experimental verification of N4. Theoretical and Computational Chemistry, 2003, , 421-439.	0.4	6
133	Computation of Franckâ€“Condon factors for many-atom systems: simulated photoelectron spectra of formic acid isotopologues. Chemical Physics, 2004, 302, 217-228.	1.9	6
134	MD Simulations Reveal Complex Water Paths in Squaleneâ€“Hopene Cyclase: Tunnel-Obstructing Mutations Increase the Flow of Water in the Active Site. ACS Omega, 2017, 2, 8495-8506.	3.5	6
135	Generation of soluble oligomeric Î²-amyloid species via copper catalyzed oxidation with implications for Alzheimerâ€™s disease: A DFT study. Journal of Molecular Modeling, 2010, 16, 1103-1108.	1.8	5
136	â€œAdapted Linear Interaction Energyâ€• A Structure-Based LIE Parametrization for Fast Prediction of Proteinâ€“Ligand Affinities. Journal of Chemical Theory and Computation, 2013, 9, 1230-1239.	5.3	5
137	Fragment molecular orbital study of the cAMP-dependent protein kinase catalyzed phosphoryl transfer: a comparison with the differential transition state stabilization method. Physical Chemistry Chemical Physics, 2016, 18, 15153-15161.	2.8	5
138	Improving the Stability of Trinitramide by Chemical Substitution: N(NF₂)₃ has Higher Stability and Excellent Propulsion Performance. Propellants, Explosives, Pyrotechnics, 2021, 46, 245-252.	1.6	4
139	Binder Materials for Green Propellants. , 2014, , 205-234.		3
140	Acetic acid conversion to ketene on Cu2O(1 0 0): Reaction mechanism deduced from experimental observations and theoretical computations. Journal of Catalysis, 2021, 402, 154-165.	6.2	3
141	Two potential energetic compounds: Ammonium superoxide and ammonium ozonide. Journal of Energetic Materials, 2000, 18, 89-95.	2.0	1
142	Chemical Reactivity: The Molecular Surface Property Approach: A Guide to Chemical Interactions in Chemistry, Medicine, and Material Science (Adv. Theory Simul. 1/2019). Advanced Theory and Simulations, 2019, 2, 1970003.	2.8	1