Johannes KÃ¤stner

List of Publications by Year
in descending order

148	7,013	81743 39	66788 78
papers	citations	h-index	g-index

153	153	153	6536
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Asymmetric Hydroboration of Ketones by Cooperative Lewis Acidâ€“Onium Salt Catalysis: A Quantum Chemical and Microkinetic Study to Combine Theory and Experiment. ACS Catalysis, 2022, 12, 1497-1507.	5.5	4
2	Status and Direction of Atom Probe Analysis of Frozen Liquids. Microscopy and Microanalysis, 2022, 28, 1150-1167.	0.2	8
3	Predicting properties of periodic systems from cluster data: A case study of liquid water. Journal of Chemical Physics, 2022, 156, 114103.	1.2	13
4	Influence of layer slipping on adsorption of light gases in covalent organic frameworks: A combined experimental and computational study. Microporous and Mesoporous Materials, 2022, 336, 111796.	2.2	6
5	Neural-network assisted study of nitrogen atom dynamics on amorphous solid water â€“ II. Diffusion. Monthly Notices of the Royal Astronomical Society, 2022, 510, 3063-3070.	1.6	5
6	Thermally Averaged Magnetic Anisotropy Tensors via Machine Learning Based on Gaussian Moments. Journal of Chemical Theory and Computation, 2022, 18, 1-12.	2.3	10
7	Hydrogen abstraction reactions in formic and thioformic acid isomers by hydrogen and deuterium atoms. Astronomy and Astrophysics, 2022, 663, A41.	2.1	9
8	Stable Cycling of Roomâ€Temperature Sodiumâ€Sulfur Batteries Based on an In Situ Crosslinked Gel Polymer Electrolyte. Advanced Functional Materials, 2022, 32, .	7.8	14
9	Rutheniumâ€Catalyzed Secondary Amine Formation Studied by Density Functional Theory. ChemCatChem, 2021, 13, 1383-1388.	1.8	1
10	Highly Active Cooperative Lewis Acidâ€”Ammonium Salt Catalyst for the Enantioselective Hydroboration of Ketones. Angewandte Chemie - International Edition, 2021, 60, 5544-5553.	7.2	16
11	New copper(II) complexes with (Z)-Nâ€²-{(2-hydroxynaphthalen-1-yl}methylene)acetohydrazide]: X-ray structure, Hirshfeld analysis, X-band electron paramagnetic resonance spectra, TD-DFT calculations and superoxide dismutase mimetic activity. Polyhedron, 2021, 195, 114969.	1.0	10
12	Highly Active Cooperative Lewis Acidâ€”Ammonium Salt Catalyst for the Enantioselective Hydroboration of Ketones. Angewandte Chemie, 2021, 133, 5604-5613.	1.6	10
13	Computational Study of the Hydrogenation Sequence of the Phosphorous Atom on Interstellar Dust Grains. Astrophysical Journal, 2021, 910, 55.	1.6	15
14	Binding energies and sticking coefficients of H₂ on crystalline and amorphous CO ice. Astronomy and Astrophysics, 2021, 648, A84.	2.1	9
15	Exploration of transferable and uniformly accurate neural network interatomic potentials using optimal experimental design. Machine Learning: Science and Technology, 2021, 2, 035009.	2.4	7
16	Hydrogenation of small aromatic heterocycles at low temperatures. Monthly Notices of the Royal Astronomical Society, 2021, 505, 3157-3164.	1.6	13
17	3D sub-nanometer analysis of glucose in an aqueous solution by cryo-atom probe tomography. Scientific Reports, 2021, 11, 11607.	1.6	10
18	Strategies for the construction of machine-learning potentials for accurate and efficient atomic-scale simulations. Machine Learning: Science and Technology, 2021, 2, 031001.	2.4	42

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19	Exploration of the Activation Mechanism of the Epigenetic Regulator MLL3: A QM/MM Study. Biomolecules, 2021, 11, 1051.	1.8	3
20	Geometry Optimization in Internal Coordinates Based on Gaussian Process Regression: Comparison of Two Approaches. Journal of Chemical Theory and Computation, 2021, 17, 5955-5967.	2.3	17
21	Quantitative Distinction between Noble Metals Located in Mesopores from Those on the External Surface. Chemistry - A European Journal, 2021, 27, 17012-17023.	1.7	11
22	Interlayer Interactions as Design Tool for Large-Pore COFs. Journal of the American Chemical Society, 2021, 143, 15711-15722.	6.6	60
23	Fast and Sample-Efficient Interatomic Neural Network Potentials for Molecules and Materials Based on Gaussian Moments. Journal of Chemical Theory and Computation, 2021, 17, 6658-6670.	2.3	14
24	Interplay of Polarity and Confinement in Asymmetric Catalysis with Chiral Rh Diene Complexes in Microemulsions. Chemistry - A European Journal, 2021, 27, 16853-16870.	1.7	3
25	A sodium bis(perfluoropinacol) borate-based electrolyte for stable, high-performance room temperature sodium-sulfur batteries based on sulfurized poly(acrylonitrile). Electrochemistry Communications, 2021, 132, 107137.	2.3	12
26	Carbon Atom Reactivity with Amorphous Solid Water: H₂O-Catalyzed Formation of H₂CO. Journal of Physical Chemistry Letters, 2021, 12, 10854-10860.	2.1	17
27	Tungsten Sulfido Alkylidene and Cationic Tungsten Sulfido Alkylidene N-Heterocyclic Carbene Complexes. Organometallics, 2021, 40, 4026-4034.	1.1	2
28	Frontispiece: Interplay of Polarity and Confinement in Asymmetric Catalysis with Chiral Rh Diene Complexes in Microemulsions. Chemistry - A European Journal, 2021, 27, .	1.7	0
29	Evaporation and Fragmentation of Organic Molecules in Strong Electric Fields Simulated with DFT. Journal of Physical Chemistry A, 2020, 124, 8633-8642.	1.1	7
30	Gaussian Moments as Physically Inspired Molecular Descriptors for Accurate and Scalable Machine Learning Potentials. Journal of Chemical Theory and Computation, 2020, 16, 5410-5421.	2.3	51
31	Isomers in Interstellar Environments. I. The Case of Z- and E-cyanomethanimine. Astrophysical Journal, 2020, 897, 158.	1.6	25
32	Charge Distribution in Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Complexes: A Combined X-ray, XAS, XES, DFT, MÃ¶ssbauer, and Catalysis Approach. ACS Catalysis, 2020, 10, 14810-14823.	5.5	19
33	Reaction Mechanism of Ring-Closing Metathesis with a Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Catalyst. Organometallics, 2020, 39, 3146-3159.	1.1	2
34	Experimental and Theoretical Study on the Role of Monomeric vs Dimeric Rhodium Oxazolidinone Norbornadiene Complexes in Catalytic Asymmetric 1,2- and 1,4-Additions. Organometallics, 2020, 39, 3131-3145.	1.1	10
35	Neural-network assisted study of nitrogen atom dynamics on amorphous solid water â€“ I. adsorptionÂand desorption. Monthly Notices of the Royal Astronomical Society, 2020, 499, 1373-1384.	1.6	18
36	Field evaporation and atom probe tomography of pure water tips. Scientific Reports, 2020, 10, 20271.	1.6	22

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37	Gas-phase spectroscopic characterization of neutral and ionic polycyclic aromatic phosphorus heterocycles (PAPHs). Monthly Notices of the Royal Astronomical Society, 2020, 500, 2564-2576.	1.6	7
38	A cryogenic ice setup to simulate carbon atom reactions in interstellar ices. Review of Scientific Instruments, 2020, 91, 054501.	0.6	17
39	Comment on â€œComputational evidence for sulfur atom tunneling in the ring flipping reaction of S4N4â€• Chemical Physics Letters, 2020, 754, 137678.	1.2	7
40	Adsorption of H₂on amorphous solid water studied with molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 7552-7563.	1.3	15
41	Revisiting the reactivity between HCO and CH3 on interstellar grain surfaces. Monthly Notices of the Royal Astronomical Society, 2020, 493, 2523-2527.	1.6	25
42	Hessian Matrix Update Scheme for Transition State Search Based on Gaussian Process Regression. Journal of Chemical Theory and Computation, 2020, 16, 5083-5089.	2.3	24
43	Efficient Production of S₈ in Interstellar Ices: The Effects of Cosmic-Ray-driven Radiation Chemistry and Nondiffusive Bulk Reactions. Astrophysical Journal, 2020, 888, 52.	1.6	45
44	Efficient training of ANN potentials by including atomic forces via Taylor expansion and application to water and a transition-metal oxide. Npj Computational Materials, 2020, 6, .	3.5	40
45	The role of atom tunneling in gas-phase reactions in planet-forming disks. Astronomy and Astrophysics, 2019, 627, A45.	2.1	3
46	The Case of H₂C₃O Isomers, Revisited: Solving the Mystery of the Missing Propadienone. Astrophysical Journal, 2019, 878, 80.	1.6	32
47	Gaussian Process Regression for Minimum Energy Path Optimization and Transition State Search. Journal of Physical Chemistry A, 2019, 123, 9600-9611.	1.1	23
48	Molybdenum and Tungsten Alkylidyne Complexes Containing Mono-, Bi-, and Tridentate N-Heterocyclic Carbenes. Organometallics, 2019, 38, 4133-4146.	1.1	30
49	Low-Temperature Kinetic Isotope Effects in CH₃OH + H â†’ CH₂OH + H₂ Shed Light on the Deuteration of Methanol in Space. Journal of Physical Chemistry A, 2019, 123, 9061-9068.	1.1	13
50	Instanton rate constant calculations using interpolated potential energy surfaces in nonredundant, rotationally and translationally invariant coordinates. Journal of Computational Chemistry, 2019, 40, 866-874.	1.5	10
51	Alcohols on the Rocks: Solid-State Formation in a H₃CCâ‰¡CH + OH Cocktail under Dark Cloud Conditions. ACS Earth and Space Chemistry, 2019, 3, 986-999.	1.2	13
52	Copper coordination in formylglycine generating enzymes. European Physical Journal: Special Topics, 2019, 227, 1657-1664.	1.2	5
53	Formation of Acetaldehyde on CO-Rich Ices. ACS Earth and Space Chemistry, 2019, 3, 958-963.	1.2	25
54	Particle methods in natural science and engineering. European Physical Journal: Special Topics, 2019, 227, 1493-1499.	1.2	2

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55	Unfolding of DNA by co-solutes: insights from Kirkwoodâ€“Buff integrals and transfer free energies. European Physical Journal: Special Topics, 2019, 227, 1665-1679.	1.2	18
56	Vibrational analysis of methyl cationâ€”Rare gas atom complexes: CH3+â€”Rg (Rg = He, Ne, Ar, Kr). Journal of Chemical Physics, 2019, 150, 084306.	1.2	11
57	Radiation chemistry in astrochemical models: From the laboratory to the ISM. Proceedings of the International Astronomical Union, 2019, 15, 454-455.	0.0	0
58	Silicate-mediated interstellar water formation: a theoretical study. Monthly Notices of the Royal Astronomical Society, 2019, 482, 5389-5400.	1.6	22
59	Proton Affinities of N-Heterocyclic Olefins and Their Implications for Organocatalyst Design. Journal of Organic Chemistry, 2019, 84, 2209-2218.	1.7	36
60	Asymmetric Carboxycyanation of Aldehydes by Cooperative AlF/Onium Salt Catalysts: from Cyanoformate to KCN as Cyanide Source. Chemistry - A European Journal, 2019, 25, 1515-1524.	1.7	17
61	Free energy reaction root mapping of alanine tripeptide in water. Molecular Physics, 2019, 117, 2284-2292.	0.8	4
62	HOCO formation in astrochemical environments by radical-induced H-abstraction from formic acid. Monthly Notices of the Royal Astronomical Society, 2019, 482, 293-300.	1.6	4
63	Gaussian process regression for geometry optimization. Journal of Chemical Physics, 2018, 148, .	1.2	81
64	Dual-Level Approach to Instanton Theory. Journal of Chemical Theory and Computation, 2018, 14, 1865-1872.	2.3	18
65	Potential energy surface interpolation with neural networks for instanton rate calculations. Journal of Chemical Physics, 2018, 148, 094106.	1.2	23
66	Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. ChemCatChem, 2018, 10, 1052-1063.	1.8	14
67	Double Regioselective Asymmetric Câ€Allylation of Isoxazolinones: Iridiumâ€Catalyzed Nâ€Allylation Followed by an Azaâ€Cope Rearrangement. Angewandte Chemie - International Edition, 2018, 57, 1404-1408.	7.2	71
68	Calculation of Reaction Rate Constants in the Canonical and Microcanonical Ensemble. Journal of Chemical Theory and Computation, 2018, 14, 5489-5498.	2.3	13
69	Gaussian Process Regression for Transition State Search. Journal of Chemical Theory and Computation, 2018, 14, 5777-5786.	2.3	48
70	Tunnelling dominates the reactions of hydrogen atoms with unsaturated alcohols and aldehydes in the dense medium. Astronomy and Astrophysics, 2018, 617, A25.	2.1	9
71	The Lewis Pair Polymerization of Lactones Using Metal Halides and N-Heterocyclic Olefins: Theoretical Insights. Molecules, 2018, 23, 432.	1.7	27
72	Hydrogen transfer reactions of interstellar complex organic molecules. Monthly Notices of the Royal Astronomical Society, 2018, 479, 2007-2015.	1.6	29

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73	Ein Aluminiumâ€Fluoridâ€Komplex mit gekoppelter Ammoniumâ€Einheit als auÃŸergewÃ¶hnlich aktiver kooperativer Katalysator in der asymmetrischen Carboxycyanierung von Aldehyden. Angewandte Chemie, 2017, 129, 4115-4119.	1.6	12
74	An Aluminum Fluoride Complex with an Appended Ammonium Salt as an Exceptionally Active Cooperative Catalyst for the Asymmetric Carboxycyanation of Aldehydes. Angewandte Chemie - International Edition, 2017, 56, 4056-4060.	7.2	32
75	Catalytic Mechanism of Salicylate Dioxygenase: QM/MM Simulations Reveal the Origin of Unexpected Regioselectivity of the Ring Cleavage. Chemistry - A European Journal, 2017, 23, 8949-8962.	1.7	17
76	Asymmetric Ketone Reduction by Imine Reductases. ChemBioChem, 2017, 18, 253-256.	1.3	50
77	On the Accessible Reaction Channels of Vinyl Gold(I) Species: Ï€â€•and Ïƒâ€Pathways. Chemistry - A European Journal, 2017, 23, 10901-10905.	1.7	44
78	Atom Tunneling in the Hydroxylation Process of Taurine/Î±-Ketoglutarate Dioxygenase Identified by Quantum Mechanics/Molecular Mechanics Simulations. Journal of Physical Chemistry B, 2017, 121, 5347-5354.	1.2	34
79	Rate constants from instanton theory via a microcanonical approach. Journal of Chemical Physics, 2017, 146, 074105.	1.2	23
80	Hydrogenation and Deuteration of C₂H₂ and C₂H₄ on Cold Grains: A Clue to the Formation Mechanism of C₂H₆ with Astronomical Interest. Astrophysical Journal, 2017, 837, 155.	1.6	26
81	Influence of Surface and Bulk Water Ice on the Reactivity of a Water-forming Reaction. Astrophysical Journal, 2017, 846, 43.	1.6	26
82	C(sp³)â^'H Bond Activation by Vinylidene Gold(I) Complexes: Aâ€‰Concerted Asynchronous or Stepwise Process?. Chemistry - A European Journal, 2017, 23, 16097-16103.	1.7	32
83	High Oxidation State Molybdenum Nâ€Heterocyclic Carbene Alkylidyne Complexes: Synthesis, Mechanistic Studies, and Reactivity. Chemistry - A European Journal, 2017, 23, 15484-15490.	1.7	38
84	Atom Tunneling in the Water Formation Reaction H₂ + OH â†' H₂O + H on an Ice Surface. ACS Earth and Space Chemistry, 2017, 1, 399-410.	1.2	38
85	Instanton rate constant calculations close to and above the crossover temperature. Journal of Computational Chemistry, 2017, 38, 2570-2580.	1.5	22
86	Comparison of classical reaction paths and tunneling paths studied with the semiclassical instanton theory. Physical Chemistry Chemical Physics, 2017, 19, 23085-23094.	1.3	12
87	Tunneling Rate Constants for H₂CO+H on Amorphous Solid Water Surfaces. Astrophysical Journal, 2017, 850, 118.	1.6	26
88	Tunneling Reaction Kinetics for the Hydrogen Abstraction Reaction H + H₂S â†' H₂ + HS in the Interstellar Medium. Journal of Physical Chemistry A, 2017, 121, 9736-9741.	1.1	24
89	Importance of tunneling in H-abstraction reactions by OH radicals. Astronomy and Astrophysics, 2017, 599, A132.	2.1	15
90	Gold(I) Vinylidene Complexes as Reactive Intermediates and Their Tendency to Ï€â€Backbond. Chemistry - A European Journal, 2016, 22, 2892-2895.	1.7	65

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91	Synergistic Substrate and Oxygen Activation in Salicylate Dioxygenase Revealed by QM/MM Simulations. Angewandte Chemie - International Edition, 2016, 55, 1168-1172.	7.2	33
92	Atom Tunneling in Chemistry. Angewandte Chemie - International Edition, 2016, 55, 5400-5413.	7.2	175
93	Reaction rates and kinetic isotope effects of H2 + OH â† H2O + H. Journal of Chemical Physics, 2016, 144, 174303.	1.2	29
94	Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction H + H₂O₂ â† H₂O + OH. Physical Chemistry Chemical Physics, 2016, 18, 33021-33030.	1.3	36
95	Formation of the prebiotic molecule NH₂CHO on astronomical amorphous solid water surfaces: accurate tunneling rate calculations. Physical Chemistry Chemical Physics, 2016, 18, 29278-29285.	1.3	67
96	Der Tunneleffekt von Atomen in der Chemie. Angewandte Chemie, 2016, 128, 5488-5502.	1.6	31
97	QM/MMâ€Simulationen ergeben synergetische Substratâ€•und Sauerstoffaktivierung in Salicylatâ€Dioxygenase. Angewandte Chemie, 2016, 128, 1182-1187.	1.6	6
98	Atom tunnelling in the reaction NH₃⁺ + H₂ â† NH₄⁺ + H and its astrochemical relevance. Faraday Discussions, 2016, 195, 69-80.	1.6	15
99	Theoretical exploration of seleno and tellurophenols as promising alternatives to sulfur ligands for anchoring to gold (111) materials. RSC Advances, 2016, 6, 4458-4468.	1.7	8
100	N₂ Binding to the FeMoâ€Cofactor of Nitrogenase. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 118-122.	0.6	34
101	An anionic molybdenum amidato bisalkyl alkylidyne complex. Journal of Organometallic Chemistry, 2015, 799-800, 223-225.	0.8	4
102	Influence of the Environment on the Oxidative Deamination of p-Substituted Benzylamines in Monoamine Oxidase. Journal of Physical Chemistry B, 2015, 119, 3678-3686.	1.2	24
103	The Stabilizing Effects in Gold Carbene Complexes. Angewandte Chemie - International Edition, 2015, 54, 10336-10340.	7.2	103
104	Reaction Mechanism of the Bicopper Enzyme Peptidylglycine Î±-Hydroxylating Monooxygenase. Journal of Biological Chemistry, 2014, 289, 13726-13738.	1.6	30
105	Nudged-elastic band used to find reaction coordinates based on the free energy. Journal of Chemical Physics, 2014, 140, 074109.	1.2	30
106	Theory and simulation of atom tunneling in chemical reactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 158-168.	6.2	83
107	Tunneling Above the Crossover Temperature. Journal of Physical Chemistry A, 2014, 118, 78-82.	1.1	28
108	<scp>C</scp>hem<scp>S</scp>hellâ€”a modular software package for <scp>QM</scp>/<scp>MM</scp> simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 101-110.	6.2	351

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109	Fe or Feï£¿NO Catalysis? A Quantum Chemical Investigation of the [Fe(CO)₃(NO)]^{â^'}â€Catalyzed Clokeâ€“Wilson Rearrangement. Chemistry - A European Journal, 2014, 20, 7254-7257.	1.7	41
110	Averaging Techniques for Reaction Barriers in QM/MM Simulations. ChemPhysChem, 2014, 15, 3264-3269.	1.0	35
111	Carbonylation of alkyl halides with [Fe(CO)3(NO)]â^': in silico identification of a common intermediate. Dalton Transactions, 2013, 42, 7519.	1.6	14
112	How maltose influences structural changes to bind to maltoseâ€binding protein: Results from umbrella sampling simulation. Proteins: Structure, Function and Bioinformatics, 2013, 81, 185-198.	1.5	19
113	Path Length Determines the Tunneling Decay of Substituted Carbenes. Chemistry - A European Journal, 2013, 19, 8207-8212.	1.7	38
114	A New Tabu-Search-Based Algorithm for Solvation of Proteins. Journal of Chemical Theory and Computation, 2013, 9, 814-821.	2.3	11
115	Reaction Mechanism of Monoamine Oxidase from QM/MM Calculations. Journal of Physical Chemistry B, 2013, 117, 14238-14246.	1.2	62
116	A Quadratically-Converging Nudged Elastic Band Optimizer. Journal of Chemical Theory and Computation, 2013, 9, 3498-3504.	2.3	16
117	Umbrella integration with higher-order correction terms. Journal of Chemical Physics, 2012, 136, 234102.	1.2	14
118	Role of Tunneling in the Enzyme Glutamate Mutase. Journal of Physical Chemistry B, 2012, 116, 13682-13689.	1.2	52
119	Are different stoichiometries feasible for complexes between lymphotoxin-alpha and tumor necrosis factor receptor 1?. BMC Structural Biology, 2012, 12, 8.	2.3	4
120	An algorithm to find minimum free-energy paths using umbrella integration. Journal of Chemical Physics, 2012, 137, 034105.	1.2	18
121	The Fragmentationâ€“Recombination Mechanism of the Enzyme Glutamate Mutase Studied by QM/MM Simulations. Journal of the American Chemical Society, 2011, 133, 10195-10203.	6.6	32
122	Deuterium Enrichment of Interstellar Methanol Explained by Atom Tunneling. Journal of Physical Chemistry A, 2011, 115, 10767-10774.	1.1	53
123	Locating Instantons in Many Degrees of Freedom. Journal of Chemical Theory and Computation, 2011, 7, 690-698.	2.3	105
124	Theoretische Chemie 2010. Nachrichten Aus Der Chemie, 2011, 59, 284-290.	0.0	0
125	Umbrella sampling. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 932-942.	6.2	901
126	Kinetic isotope effects calculated with the instanton method. Journal of Computational Chemistry, 2011, 32, 3456-3463.	1.5	35

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127	Adaptive integration grids in instanton theory improve the numerical accuracy at low temperature. Journal of Chemical Physics, 2011, 134, 184107.	1.2	65
128	Human Epidermal Growth Factor Receptor (EGFR) Aligned on the Plasma Membrane Adopts Key Features of Drosophila EGFR Asymmetry. Molecular and Cellular Biology, 2011, 31, 2241-2252.	1.1	37
129	Innentitelbild: Tunneln von Wasserstoffatomen kann zur Bildung von H2 im Weltraum beitragen (Angew. Chem. 40/2010). Angewandte Chemie, 2010, 122, 7296-7296.	1.6	0
130	Hydrogenâ€Atom Tunneling Could Contribute to H₂ Formation in Space. Angewandte Chemie - International Edition, 2010, 49, 7350-7352.	7.2	73
131	Inside Cover: Hydrogen-Atom Tunneling Could Contribute to H2 Formation in Space (Angew. Chem. Int.) Tj ETQq1 1 0.784314 rgBT /Ov	7.2	1
132	The ribosome catalyzes peptide bond formation by providing high ionic strength. Molecular Physics, 2010, 108, 293-306.	0.8	21
133	Umbrella integration in two or more reaction coordinates. Journal of Chemical Physics, 2009, 131, 034109.	1.2	49
134	An embedded cluster study of the formation of water on interstellar dust grains. Physical Chemistry Chemical Physics, 2009, 11, 5431.	1.3	78
135	Ectodomain orientation, conformational plasticity and oligomerization of ErbB1 receptors investigated by molecular dynamics. Journal of Structural Biology, 2009, 167, 117-128.	1.3	42
136	DL-FIND: An Open-Source Geometry Optimizer for Atomistic Simulations. Journal of Physical Chemistry A, 2009, 113, 11856-11865.	1.1	466
137	Finite-temperature effects in enzymatic reactions â€" Insights from QM/MM free-energy simulations. Canadian Journal of Chemistry, 2009, 87, 1322-1337.	0.6	64
138	Superlinearly converging dimer method for transition state search. Journal of Chemical Physics, 2008, 128, 014106.	1.2	282
139	Exploiting QM/MM Capabilities in Geometry Optimization:â€‰ A Microiterative Approach Using Electrostatic Embedding. Journal of Chemical Theory and Computation, 2007, 3, 1064-1072.	2.3	48
140	Ammonia Production at the FeMo Cofactor of Nitrogenase:â€‰ Results from Density Functional Theory. Journal of the American Chemical Society, 2007, 129, 2998-3006.	6.6	125
141	QM/MM Free-Energy Perturbation Compared to Thermodynamic Integration and Umbrella Sampling:â€‰ Application to an Enzymatic Reaction. Journal of Chemical Theory and Computation, 2006, 2, 452-461.	2.3	152
142	Analysis of the statistical error in umbrella sampling simulations by umbrella integration. Journal of Chemical Physics, 2006, 124, 234106.	1.2	150
143	Bridging the gap between thermodynamic integration and umbrella sampling provides a novel analysis method: â€œUmbrella integrationâ€. Journal of Chemical Physics, 2005, 123, 144104.	1.2	342
144	Towards an Understanding of the Workings of Nitrogenase from DFT Calculations. ChemPhysChem, 2005, 6, 1724-1726.	1.0	45

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145	Activation and protonation of dinitrogen at the FeMo cofactor of nitrogenase. Journal of Chemical Physics, 2005, 123, 074306.	1.2	49
146	Model for Acetylene Reduction by Nitrogenase Derived from Density Functional Theory. Inorganic Chemistry, 2005, 44, 4568-4575.	1.9	32
147	Projector augmented wave method:ab initio molecular dynamics with full wave functions. Bulletin of Materials Science, 2003, 26, 33-41.	0.8	374
148	Nitrogen Binding to the FeMo-Cofactor of Nitrogenase. Journal of the American Chemical Society, 2003, 125, 15772-15778.	6.6	109