Johannes KÃ¤stner

List of Publications by Year
in descending order

148	7,013	81839	66879
papers	citations	39 h-index	78 g-index

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

#	Article	IF	Citations
1	Umbrella sampling. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 932-942.	6.2	901
2	DL-FIND: An Open-Source Geometry Optimizer for Atomistic Simulations. Journal of Physical Chemistry A, 2009, 113, 11856-11865.	1.1	466
3	Projector augmented wave method:ab initio molecular dynamics with full wave functions. Bulletin of Materials Science, 2003, 26, 33-41.	0.8	374
4	<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
5	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
6	Superlinearly converging dimer method for transition state search. Journal of Chemical Physics, 2008, 128, 014106.	1.2	282
7	Atom Tunneling in Chemistry. Angewandte Chemie - International Edition, 2016, 55, 5400-5413.	7.2	175
8	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
9	Analysis of the statistical error in umbrella sampling simulations by umbrella integration. Journal of Chemical Physics, 2006, 124, 234106.	1.2	150
10	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
11	Nitrogen Binding to the FeMo-Cofactor of Nitrogenase. Journal of the American Chemical Society, 2003, 125, 15772-15778.	6.6	109
12	Locating Instantons in Many Degrees of Freedom. Journal of Chemical Theory and Computation, 2011, 7, 690-698.	2.3	105
13	The Stabilizing Effects in Gold Carbene Complexes. Angewandte Chemie - International Edition, 2015, 54, 10336-10340.	7.2	103
14	Theory and simulation of atom tunneling in chemical reactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 158-168.	6.2	83
15	Gaussian process regression for geometry optimization. Journal of Chemical Physics, 2018, 148, .	1.2	81
16	An embedded cluster study of the formation of water on interstellar dust grains. Physical Chemistry Chemical Physics, 2009, 11, 5431.	1.3	78
17	Hydrogenâ€Atom Tunneling Could Contribute to H₂ Formation in Space. Angewandte Chemie - International Edition, 2010, 49, 7350-7352.	7.2	73
18	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

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19	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
20	Adaptive integration grids in instanton theory improve the numerical accuracy at low temperature. Journal of Chemical Physics, 2011, 134, 184107.	1.2	65
21	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
22	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
23	Reaction Mechanism of Monoamine Oxidase from QM/MM Calculations. Journal of Physical Chemistry B, 2013, 117, 14238-14246.	1.2	62
24	Interlayer Interactions as Design Tool for Large-Pore COFs. Journal of the American Chemical Society, 2021, 143, 15711-15722.	6.6	60
25	Deuterium Enrichment of Interstellar Methanol Explained by Atom Tunneling. Journal of Physical Chemistry A, 2011, 115, 10767-10774.	1.1	53
26	Role of Tunneling in the Enzyme Glutamate Mutase. Journal of Physical Chemistry B, 2012, 116, 13682-13689.	1.2	52
27	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
28	Asymmetric Ketone Reduction by Imine Reductases. ChemBioChem, 2017, 18, 253-256.	1.3	50
29	Activation and protonation of dinitrogen at the FeMo cofactor of nitrogenase. Journal of Chemical Physics, 2005, 123, 074306.	1.2	49
30	Umbrella integration in two or more reaction coordinates. Journal of Chemical Physics, 2009, 131, 034109.	1.2	49
31	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
32	Gaussian Process Regression for Transition State Search. Journal of Chemical Theory and Computation, 2018, 14, 5777-5786.	2.3	48
33	Towards an Understanding of the Workings of Nitrogenase from DFT Calculations. ChemPhysChem, 2005, 6, 1724-1726.	1.0	45
34	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
35	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
36	Ectodomain orientation, conformational plasticity and oligomerization of ErbB1 receptors investigated by molecular dynamics. Journal of Structural Biology, 2009, 167, 117-128.	1.3	42

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37	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
38	Fe or Feï£¿NO Catalysis? A Quantum Chemical Investigation of the [Fe(CO)₃(NO)]^{â^'}â€Catalyzed Cloke–Wilson Rearrangement. Chemistry - A European Journal, 2014, 20, 7254-7257.	1.7	41
39	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
40	Path Length Determines the Tunneling Decay of Substituted Carbenes. Chemistry - A European Journal, 2013, 19, 8207-8212.	1.7	38
41	High Oxidation State Molybdenum N–Heterocyclic Carbene Alkylidyne Complexes: Synthesis, Mechanistic Studies, and Reactivity. Chemistry - A European Journal, 2017, 23, 15484-15490.	1.7	38
42	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
43	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
44	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
45	Proton Affinities of N-Heterocyclic Olefins and Their Implications for Organocatalyst Design. Journal of Organic Chemistry, 2019, 84, 2209-2218.	1.7	36
46	Kinetic isotope effects calculated with the instanton method. Journal of Computational Chemistry, 2011, 32, 3456-3463.	1.5	35
47	Averaging Techniques for Reaction Barriers in QM/MM Simulations. ChemPhysChem, 2014, 15, 3264-3269.	1.0	35
48	N₂ Binding to the FeMoâ€Cofactor of Nitrogenase. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 118-122.	0.6	34
49	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
50	Synergistic Substrate and Oxygen Activation in Salicylate Dioxygenase Revealed by QM/MM Simulations. Angewandte Chemie - International Edition, 2016, 55, 1168-1172.	7.2	33
51	Model for Acetylene Reduction by Nitrogenase Derived from Density Functional Theory. Inorganic Chemistry, 2005, 44, 4568-4575.	1.9	32
52	The Fragmentation–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
53	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
54	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

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55	The Case of H₂C₃O Isomers, Revisited: Solving the Mystery of the Missing Propadienone. Astrophysical Journal, 2019, 878, 80.	1.6	32
56	Der Tunneleffekt von Atomen in der Chemie. Angewandte Chemie, 2016, 128, 5488-5502.	1.6	31
57	Reaction Mechanism of the Bicopper Enzyme Peptidylglycine Î±-Hydroxylating Monooxygenase. Journal of Biological Chemistry, 2014, 289, 13726-13738.	1.6	30
58	Nudged-elastic band used to find reaction coordinates based on the free energy. Journal of Chemical Physics, 2014, 140, 074109.	1.2	30
59	Molybdenum and Tungsten Alkylidyne Complexes Containing Mono-, Bi-, and Tridentate N-Heterocyclic Carbenes. Organometallics, 2019, 38, 4133-4146.	1.1	30
60	Reaction rates and kinetic isotope effects of H2 + OH â†' H2O + H. Journal of Chemical Physics, 2016, 144, 174303.	1.2	29
61	Hydrogen transfer reactions of interstellar complex organic molecules. Monthly Notices of the Royal Astronomical Society, 2018, 479, 2007-2015.	1.6	29
62	Tunneling Above the Crossover Temperature. Journal of Physical Chemistry A, 2014, 118, 78-82.	1.1	28
63	The Lewis Pair Polymerization of Lactones Using Metal Halides and N-Heterocyclic Olefins: Theoretical Insights. Molecules, 2018, 23, 432.	1.7	27
64	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
65	Influence of Surface and Bulk Water Ice on the Reactivity of a Water-forming Reaction. Astrophysical Journal, 2017, 846, 43.	1.6	26
66	Tunneling Rate Constants for H₂CO+H on Amorphous Solid Water Surfaces. Astrophysical Journal, 2017, 850, 118.	1.6	26
67	Formation of Acetaldehyde on CO-Rich Ices. ACS Earth and Space Chemistry, 2019, 3, 958-963.	1.2	25
68	Isomers in Interstellar Environments. I. The Case of Z- and E-cyanomethanimine. Astrophysical Journal, 2020, 897, 158.	1.6	25
69	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
70	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
71	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
72	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

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73	Rate constants from instanton theory via a microcanonical approach. Journal of Chemical Physics, 2017, 146, 074105.	1.2	23
74	Potential energy surface interpolation with neural networks for instanton rate calculations. Journal of Chemical Physics, 2018, 148, 094106.	1.2	23
75	Gaussian Process Regression for Minimum Energy Path Optimization and Transition State Search. Journal of Physical Chemistry A, 2019, 123, 9600-9611.	1.1	23
76	Instanton rate constant calculations close to and above the crossover temperature. Journal of Computational Chemistry, 2017, 38, 2570-2580.	1.5	22
77	Silicate-mediated interstellar water formation: a theoretical study. Monthly Notices of the Royal Astronomical Society, 2019, 482, 5389-5400.	1.6	22
78	Field evaporation and atom probe tomography of pure water tips. Scientific Reports, 2020, 10, 20271.	1.6	22
79	The ribosome catalyzes peptide bond formation by providing high ionic strength. Molecular Physics, 2010, 108, 293-306.	0.8	21
80	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
81	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
82	An algorithm to find minimum free-energy paths using umbrella integration. Journal of Chemical Physics, 2012, 137, 034105.	1.2	18
83	Dual-Level Approach to Instanton Theory. Journal of Chemical Theory and Computation, 2018, 14, 1865-1872.	2.3	18
84	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
85	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
86	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
87	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
88	A cryogenic ice setup to simulate carbon atom reactions in interstellar ices. Review of Scientific Instruments, 2020, 91, 054501.	0.6	17
89	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
90	Carbon Atom Reactivity with Amorphous Solid Water: H₂O-Catalyzed Formation of H₂CO. Journal of Physical Chemistry Letters, 2021, 12, 10854-10860.	2.1	17

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91	A Quadratically-Converging Nudged Elastic Band Optimizer. Journal of Chemical Theory and Computation, 2013, 9, 3498-3504.	2.3	16
92	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
93	Atom tunnelling in the reaction NH₃⁺ + H₂ â† NH₄⁺ + H and its astrochemical relevance. Faraday Discussions, 2016, 195, 69-80.	1.6	15
94	Importance of tunneling in H-abstraction reactions by OH radicals. Astronomy and Astrophysics, 2017, 599, A132.	2.1	15
95	Adsorption of H₂on amorphous solid water studied with molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 7552-7563.	1.3	15
96	Computational Study of the Hydrogenation Sequence of the Phosphorous Atom on Interstellar Dust Grains. Astrophysical Journal, 2021, 910, 55.	1.6	15
97	Umbrella integration with higher-order correction terms. Journal of Chemical Physics, 2012, 136, 234102.	1.2	14
98	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
99	Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. ChemCatChem, 2018, 10, 1052-1063.	1.8	14
100	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
101	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
102	Calculation of Reaction Rate Constants in the Canonical and Microcanonical Ensemble. Journal of Chemical Theory and Computation, 2018, 14, 5489-5498.	2.3	13
103	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
104	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
105	Hydrogenation of small aromatic heterocycles at low temperatures. Monthly Notices of the Royal Astronomical Society, 2021, 505, 3157-3164.	1.6	13
106	Predicting properties of periodic systems from cluster data: A case study of liquid water. Journal of Chemical Physics, 2022, 156, 114103.	1.2	13
107	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
108	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

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109	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
110	A New Tabu-Search-Based Algorithm for Solvation of Proteins. Journal of Chemical Theory and Computation, 2013, 9, 814-821.	2.3	11
111	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
112	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
113	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
114	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
115	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
116	Highly Active Cooperative Lewis Acidâ€"Ammonium Salt Catalyst for the Enantioselective Hydroboration of Ketones. Angewandte Chemie, 2021, 133, 5604-5613.	1.6	10
117	3D sub-nanometer analysis of glucose in an aqueous solution by cryo-atom probe tomography. Scientific Reports, 2021, 11, 11607.	1.6	10
118	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
119	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
120	Binding energies and sticking coefficients of H₂ on crystalline and amorphous CO ice. Astronomy and Astrophysics, 2021, 648, A84.	2.1	9
121	Hydrogen abstraction reactions in formic and thioformic acid isomers by hydrogen and deuterium atoms. Astronomy and Astrophysics, 2022, 663, A41.	2.1	9
122	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
123	Status and Direction of Atom Probe Analysis of Frozen Liquids. Microscopy and Microanalysis, 2022, 28, 1150-1167.	0.2	8
124	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
125	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
126	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

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127	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
128	QM/MMâ€Simulationen ergeben synergetische Substratâ€•und Sauerstoffaktivierung in Salicylatâ€Dioxygenase. Angewandte Chemie, 2016, 128, 1182-1187.	1.6	6
129	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
130	Copper coordination in formylglycine generating enzymes. European Physical Journal: Special Topics, 2019, 227, 1657-1664.	1.2	5
131	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
132	Are different stoichiometries feasible for complexes between lymphotoxin-alpha and tumor necrosis factor receptor 1?. BMC Structural Biology, 2012, 12, 8.	2.3	4
133	An anionic molybdenum amidato bisalkyl alkylidyne complex. Journal of Organometallic Chemistry, 2015, 799-800, 223-225.	0.8	4
134	Free energy reaction root mapping of alanine tripeptide in water. Molecular Physics, 2019, 117, 2284-2292.	0.8	4
135	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
136	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
137	The role of atom tunneling in gas-phase reactions in planet-forming disks. Astronomy and Astrophysics, 2019, 627, A45.	2.1	3
138	Exploration of the Activation Mechanism of the Epigenetic Regulator MLL3: A QM/MM Study. Biomolecules, 2021, 11, 1051.	1.8	3
139	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
140	Particle methods in natural science and engineering. European Physical Journal: Special Topics, 2019, 227, 1493-1499.	1.2	2
141	Reaction Mechanism of Ring-Closing Metathesis with a Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Catalyst. Organometallics, 2020, 39, 3146-3159.	1.1	2
142	Tungsten Sulfido Alkylidene and Cationic Tungsten Sulfido Alkylidene N-Heterocyclic Carbene Complexes. Organometallics, 2021, 40, 4026-4034.	1.1	2
143	Inside Cover: Hydrogen-Atom Tunneling Could Contribute to H2 Formation in Space (Angew. Chem. Int.) Tj ETQq1 1 0.784314 rgBT /O	7.2	1
144	Rutheniumâ€Catalyzed Secondary Amine Formation Studied by Density Functional Theory. ChemCatChem, 2021, 13, 1383-1388.	1.8	1

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145	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
146	Theoretische Chemie 2010. Nachrichten Aus Der Chemie, 2011, 59, 284-290.	0.0	0
147	Radiation chemistry in astrochemical models: From the laboratory to the ISM. Proceedings of the International Astronomical Union, 2019, 15, 454-455.	0.0	0
148	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