Johannes Kstner

List of Publications by Citations

145 papers	5,227 citations	34 h-index	68 g-index
153 ext. papers	6,172 ext. citations	5.2 avg, IF	6.57 L-index

#	Paper	IF	Citations
145	Umbrella sampling. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 932-942	7.9	645
144	DL-FIND: an open-source geometry optimizer for atomistic simulations. *Journal of Physical Chemistry A*, **2009**, 113, 11856-65	2.8	356
143	Bridging the gap between thermodynamic integration and umbrella sampling provides a novel analysis method: "Umbrella integration". *Journal of Chemical Physics*, **2005**, 123, 144104	3.9	293
142	Projector augmented wave method:ab initio molecular dynamics with full wave functions. *Bulletin of Materials Science*, **2003**, 26, 33-41	1.7	274
141	ChemShell□ modular software package for QM/MM simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 101-110	7.9	267
140	Superlinearly converging dimer method for transition state search. *Journal of Chemical Physics*, **2008**, 128, 014106	3.9	220
139	QM/MM Free-Energy Perturbation Compared to Thermodynamic Integration and Umbrella Sampling: Application to an Enzymatic Reaction. *Journal of Chemical Theory and Computation*, **2006**, 2, 452-61	6.4	134
138	Analysis of the statistical error in umbrella sampling simulations by umbrella integration. *Journal of Chemical Physics*, **2006**, 124, 234106	3.9	132
137	Atom Tunneling in Chemistry. *Angewandte Chemie - International Edition*, **2016**, 55, 5400-13	16.4	124
136	Ammonia production at the FeMo cofactor of nitrogenase: results from density functional theory. *Journal of the American Chemical Society*, **2007**, 129, 2998-3006	16.4	104
135	Nitrogen binding to the FeMo-cofactor of nitrogenase. *Journal of the American Chemical Society*, **2003**, 125, 15772-8	16.4	102
134	Locating Instantons in Many Degrees of Freedom. *Journal of Chemical Theory and Computation*, **2011**, 7, 690-8	6.4	94
133	The Stabilizing Effects in Gold Carbene Complexes. *Angewandte Chemie - International Edition*, **2015**, 54, 10336-40	16.4	85
132	Theory and simulation of atom tunneling in chemical reactions. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 158-168	7.9	67
131	An embedded cluster study of the formation of water on interstellar dust grains. *Physical Chemistry Chemical Physics*, **2009**, 11, 5431-6	3.6	65
130	Hydrogen-atom tunneling could contribute to H2 formation in space. *Angewandte Chemie - International Edition*, **2010**, 49, 7350-2	16.4	64
129	Adaptive integration grids in instanton theory improve the numerical accuracy at low temperature. *Journal of Chemical Physics*, **2011**, 134, 184107	3.9	62

128	Finite-temperature effects in enzymatic reactions Insights from QM/MM free-energy simulations. *Canadian Journal of Chemistry*, **2009**, 87, 1322-1337	0.9	57
127	Gold(I) Vinylidene Complexes as Reactive Intermediates and Their Tendency to Backbond. *Chemistry - A European Journal*, **2016**, 22, 2892-5	4.8	57
126	Reaction mechanism of monoamine oxidase from QM/MM calculations. *Journal of Physical Chemistry B*, **2013**, 117, 14238-46	3.4	52
125	Double Regioselective Asymmetric C-Allylation of Isoxazolinones: Iridium-Catalyzed N-Allylation Followed by an Aza-Cope Rearrangement. *Angewandte Chemie - International Edition*, **2018**, 57, 1404-1408	16.4	49
124	Role of tunneling in the enzyme glutamate mutase. *Journal of Physical Chemistry B*, **2012**, 116, 13682-9	3.4	48
123	Deuterium enrichment of interstellar methanol explained by atom tunneling. *Journal of Physical Chemistry A*, **2011**, 115, 10767-74	2.8	48
122	Formation of the prebiotic molecule NHCHO on astronomical amorphous solid water surfaces: accurate tunneling rate calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 29278-29285	3.6	45
121	Umbrella integration in two or more reaction coordinates. *Journal of Chemical Physics*, **2009**, 131, 034109	3.9	45
120	Gaussian process regression for geometry optimization. *Journal of Chemical Physics*, **2018**, 148, 094114	3.9	44
119	Exploiting QM/MM Capabilities in Geometry Optimization: A Microiterative Approach Using Electrostatic Embedding. *Journal of Chemical Theory and Computation*, **2007**, 3, 1064-72	6.4	42
118	Ectodomain orientation, conformational plasticity and oligomerization of ErbB1 receptors investigated by molecular dynamics. *Journal of Structural Biology*, **2009**, 167, 117-28	3.4	39
117	Activation and protonation of dinitrogen at the FeMo cofactor of nitrogenase. *Journal of Chemical Physics*, **2005**, 123, 074306	3.9	39
116	Zu den stabilisierenden Effekten in Carbengoldkomplexen. *Angewandte Chemie*, **2015**, 127, 10477-10481	3.6	36
115	Fe or Fe-NO catalysis? A quantum chemical investigation of the [Fe(CO)3(NO)](-)-catalyzed Cloke-Wilson rearrangement. *Chemistry - A European Journal*, **2014**, 20, 7254-7	4.8	36
114	Towards an understanding of the workings of nitrogenase from DFT calculations. *ChemPhysChem*, **2005**, 6, 1724-6	3.2	36
113	Asymmetric Ketone Reduction by Imine Reductases. *ChemBioChem*, **2017**, 18, 253-256	3.8	35
112	On the Accessible Reaction Channels of Vinyl Gold(I) Species: and Pathways. *Chemistry - A European Journal*, **2017**, 23, 10901-10905	4.8	34
111	Path length determines the tunneling decay of substituted carbenes. *Chemistry - A European Journal*, **2013**, 19, 8207-12	4.8	34

110	Kinetic isotope effects calculated with the instanton method. *Journal of Computational Chemistry*, **2011**, 32, 3456-63	3.5	32
109	Human epidermal growth factor receptor (EGFR) aligned on the plasma membrane adopts key features of Drosophila EGFR asymmetry. *Molecular and Cellular Biology*, **2011**, 31, 2241-52	4.8	31
108	Averaging techniques for reaction barriers in QM/MM simulations. *ChemPhysChem*, **2014**, 15, 3264-9	3.2	30
107	Atom Tunneling in the Water Formation Reaction H2 + OH -m H2O + H on an Ice Surface. *ACS Earth and Space Chemistry*, **2017**, 1, 399-410	3.2	29
106	The fragmentation-recombination mechanism of the enzyme glutamate mutase studied by QM/MM simulations. *Journal of the American Chemical Society*, **2011**, 133, 10195-203	16.4	29
105	Model for acetylene reduction by nitrogenase derived from density functional theory. *Inorganic Chemistry*, **2005**, 44, 4568-75	5.1	29
104	High Oxidation State Molybdenum N-Heterocyclic Carbene Alkylidyne Complexes: Synthesis, Mechanistic Studies, and Reactivity. *Chemistry - A European Journal*, **2017**, 23, 15484-15490	4.8	28
103	Gaussian Process Regression for Transition State Search. *Journal of Chemical Theory and Computation*, **2018**, 14, 5777-5786	6.4	28
102	Efficient Production of S8 in Interstellar Ices: The Effects of Cosmic-Ray-driven Radiation Chemistry and Nondiffusive Bulk Reactions. *Astrophysical Journal*, **2020**, 888, 52	4.7	27
101	Tunneling above the crossover temperature. *Journal of Physical Chemistry A*, **2014**, 118, 78-82	2.8	27
100	Synergistic Substrate and Oxygen Activation in Salicylate Dioxygenase Revealed by QM/MM Simulations. *Angewandte Chemie - International Edition*, **2016**, 55, 1168-72	16.4	27
99	Hydrogen transfer reactions of interstellar complex organic molecules. *Monthly Notices of the Royal Astronomical Society*, **2018**, 479, 2007-2015	4.3	26
98	N2 Binding to the FeMo-Cofactor of Nitrogenase. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2015**, 641, 118-122	1.3	26
97	Nudged-elastic band used to find reaction coordinates based on the free energy. *Journal of Chemical Physics*, **2014**, 140, 074109	3.9	26
96	Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction H + HO -m HO + OH. *Physical Chemistry Chemical Physics*, **2016**, 18, 33021-33030	3.6	26
95	C(sp)-H Bond Activation by Vinylidene Gold(I) Complexes: A Concerted Asynchronous or Stepwise Process?. *Chemistry - A European Journal*, **2017**, 23, 16097-16103	4.8	25
94	Reaction mechanism of the bicopper enzyme peptidylglycine -hydroxylating monooxygenase. *Journal of Biological Chemistry*, **2014**, 289, 13726-38	5.4	25
93	Gaussian Moments as Physically Inspired Molecular Descriptors for Accurate and Scalable Machine Learning Potentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 5410-5421	6.4	25

92	Proton Affinities of N-Heterocyclic Olefins and Their Implications for Organocatalyst Design. *Journal of Organic Chemistry*, **2019**, 84, 2209-2218	4.2	25
91	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	16.4	24
90	Der Tunneleffekt von Atomen in der Chemie. *Angewandte Chemie*, **2016**, 128, 5488-5502	3.6	23
89	Influence of the environment on the oxidative deamination of p-substituted benzylamines in monoamine oxidase. *Journal of Physical Chemistry B*, **2015**, 119, 3678-86	3.4	23
88	Reaction rates and kinetic isotope effects of H2 + OH -rH2O + H. *Journal of Chemical Physics*, **2016**, 144, 174303	3.9	23
87	The Lewis Pair Polymerization of Lactones Using Metal Halides and N-Heterocyclic Olefins: Theoretical Insights. *Molecules*, **2018**, 23,	4.8	22
86	Influence of Surface and Bulk Water Ice on the Reactivity of a Water-forming Reaction. *Astrophysical Journal*, **2017**, 846, 43	4.7	22
85	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,	10.9	22
84	Atom Tunneling in the Hydroxylation Process of Taurine/Ketoglutarate Dioxygenase Identified by Quantum Mechanics/Molecular Mechanics Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 5347-5354	3.4	21
83	Rate constants from instanton theory via a microcanonical approach. *Journal of Chemical Physics*, **2017**, 146, 074105	3.9	21
82	Instanton rate constant calculations close to and above the crossover temperature. *Journal of Computational Chemistry*, **2017**, 38, 2570-2580	3.5	21
81	Hydrogenation and Deuteration of C2H2and C2H4on Cold Grains: A Clue to the Formation Mechanism of C2H6with Astronomical Interest. *Astrophysical Journal*, **2017**, 837, 155	4.7	19
80	The Case of H2C3O Isomers, Revisited: Solving the Mystery of the Missing Propadienone. *Astrophysical Journal*, **2019**, 878, 80	4.7	19
79	Molybdenum and Tungsten Alkylidyne Complexes Containing Mono-, Bi-, and Tridentate N-Heterocyclic Carbenes. *Organometallics*, **2019**, 38, 4133-4146	3.8	19
78	Formation of Acetaldehyde on CO-Rich Ices. *ACS Earth and Space Chemistry*, **2019**, 3, 958-963	3.2	18
77	Tunneling Reaction Kinetics for the Hydrogen Abstraction Reaction H + HS -rH + HS in the Interstellar Medium. *Journal of Physical Chemistry A*, **2017**, 121, 9736-9741	2.8	18
76	The ribosome catalyzes peptide bond formation by providing high ionic strength. *Molecular Physics*, **2010**, 108, 293-306	1.7	17
75	Unfolding of DNA by co-solutes: insights from KirkwoodBuff integrals and transfer free energies. *European Physical Journal: Special Topics*, **2019**, 227, 1665-1679	2.3	16

74	A Quadratically-Converging Nudged Elastic Band Optimizer. *Journal of Chemical Theory and Computation*, **2013**, 9, 3498-504	6.4	16
73	Interlayer Interactions as Design Tool for Large-Pore COFs. *Journal of the American Chemical Society*, **2021**, 143, 15711-15722	16.4	16
72	Revisiting the reactivity between HCO and CH3 on interstellar grain surfaces. *Monthly Notices of the Royal Astronomical Society*, **2020**, 493, 2523-2527	4.3	14
71	Potential energy surface interpolation with neural networks for instanton rate calculations. *Journal of Chemical Physics*, **2018**, 148, 094106	3.9	14
70	Gaussian Process Regression for Minimum Energy Path Optimization and Transition State Search. *Journal of Physical Chemistry A*, **2019**, 123, 9600-9611	2.8	14
69	Tunneling Rate Constants for H2CO+H on Amorphous Solid Water Surfaces. *Astrophysical Journal*, **2017**, 850, 118	4.7	14
68	Umbrella integration with higher-order correction terms. *Journal of Chemical Physics*, **2012**, 136, 234102	3.9	14
67	Field evaporation and atom probe tomography of pure water tips. *Scientific Reports*, **2020**, 10, 20271	4.9	14
66	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	4.8	13
65	Hessian Matrix Update Scheme for Transition State Search Based on Gaussian Process Regression. *Journal of Chemical Theory and Computation*, **2020**, 16, 5083-5089	6.4	13
64	Atom tunnelling in the reaction NH + H -> N + H and its astrochemical relevance. *Faraday Discussions*, **2016**, 195, 69-80	3.6	13
63	Carbonylation of alkyl halides with [Fe(CO)3(NO)]-: in silico identification of a common intermediate. *Dalton Transactions*, **2013**, 42, 7519-25	4.3	13
62	How maltose influences structural changes to bind to maltose-binding protein: results from umbrella sampling simulation. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 185-98	4.2	13
61	An algorithm to find minimum free-energy paths using umbrella integration. *Journal of Chemical Physics*, **2012**, 137, 034105	3.9	13
60	A cryogenic ice setup to simulate carbon atom reactions in interstellar ices. *Review of Scientific Instruments*, **2020**, 91, 054501	1.7	12
59	Importance of tunneling in H-abstraction reactions by OH radicals. *Astronomy and Astrophysics*, **2017**, 599, A132	5.1	12
58	Dual-Level Approach to Instanton Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 1865-1872	5.4	12
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56	Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. *ChemCatChem*, **2018**, 10, 1052-1063	5.2	11
55	A New Tabu-Search-Based Algorithm for Solvation of Proteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 814-21	6.4	11
54	Strategies for the construction of machine-learning potentials for accurate and efficient atomic-scale simulations. *Machine Learning: Science and Technology*, **2021**, 2, 031001	5.1	11
53	Calculation of Reaction Rate Constants in the Canonical and Microcanonical Ensemble. *Journal of Chemical Theory and Computation*, **2018**, 14, 5489-5498	6.4	11
52	Alcohols on the Rocks: Solid-State Formation in a H3CC?CH + OH Cocktail under Dark Cloud Conditions. *ACS Earth and Space Chemistry*, **2019**, 3, 986-999	3.2	10
51	Comparison of classical reaction paths and tunneling paths studied with the semiclassical instanton theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 23085-23094	3.6	10
50	Ein Aluminium-Fluorid-Komplex mit gekoppelter Ammonium-Einheit als außergewöhnlich aktiver kooperativer Katalysator in der asymmetrischen Carboxycyanierung von Aldehyden. *Angewandte Chemie*, **2017**, 129, 4115-4119	3.6	9
49	Tunneln von Wasserstoffatomen kann zur Bildung von H2 im Weltraum beitragen. *Angewandte Chemie*, **2010**, 122, 7508-7511	3.6	9
48	Isomers in Interstellar Environments. I. The Case of Z- and E-cyanomethanimine. *Astrophysical Journal*, **2020**, 897, 158	4.7	9
47	Charge Distribution in Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Complexes: A Combined X-ray, XAS, XES, DFT, Mössbauer, and Catalysis Approach. *ACS Catalysis*, **2020**, 10, 14810-14823	13.1	9
46	Neural-network assisted study of nitrogen atom dynamics on amorphous solid water – I. adsorption and desorption. *Monthly Notices of the Royal Astronomical Society*, **2020**, 499, 1373-1384	4.3	9
45	Silicate-mediated interstellar water formation: A theoretical study. *Monthly Notices of the Royal Astronomical Society*, **2019**, 482, 5389-5400	4.3	9
44	Low-Temperature Kinetic Isotope Effects in CHOH + H → CHOH + H Shed Light on the Deuteration of Methanol in Space. *Journal of Physical Chemistry A*, **2019**, 123, 9061-9068	2.8	8
43	Tunnelling dominates the reactions of hydrogen atoms with unsaturated alcohols and aldehydes in the dense medium. *Astronomy and Astrophysics*, **2018**, 617, A25	5.1	8
42	Comment on "Computational evidence for sulfur atom tunneling in the ring flipping reaction of S4N4". *Chemical Physics Letters*, **2020**, 754, 137678	2.5	6
41	Adsorption of H on amorphous solid water studied with molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2020**, 22, 7552-7563	3.6	6
40	Carbon Atom Reactivity with Amorphous Solid Water: HO-Catalyzed Formation of HCO. *Journal of Physical Chemistry Letters*, **2021**, 12, 10854-10860	6.4	6
39	Evaporation and Fragmentation of Organic Molecules in Strong Electric Fields Simulated with DFT. *Journal of Physical Chemistry A*, **2020**, 124, 8633-8642	2.8	6

38	Computational Study of the Hydrogenation Sequence of the Phosphorous Atom on Interstellar Dust Grains. *Astrophysical Journal*, **2021**, 910, 55	4.7	6
37	Vibrational analysis of methyl cation-Rare gas atom complexes: CH -Rg (Rg = He, Ne, Ar, Kr). *Journal of Chemical Physics*, **2019**, 150, 084306	3.9	6
36	New copper(II) complexes with (Z)-N?-{(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	2.7	6
35	Theoretical exploration of seleno and tellurophenols as promising alternatives to sulfur ligands for anchoring to gold (111) materials. *RSC Advances*, **2016**, 6, 4458-4468	3.7	5
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	3.8	5
33	Highly Active Cooperative Lewis Acid-Ammonium Salt Catalyst for the Enantioselective Hydroboration of Ketones. *Angewandte Chemie - International Edition*, **2021**, 60, 5544-5553	16.4	5
32	Instanton rate constant calculations using interpolated potential energy surfaces in nonredundant, rotationally and translationally invariant coordinates. *Journal of Computational Chemistry*, **2019**, 40, 866-874	3.5	4
31	QM/MM-Simulationen ergeben synergetische Substrat- und Sauerstoffaktivierung in Salicylat-Dioxygenase. *Angewandte Chemie*, **2016**, 128, 1182-1187	3.6	4
30	An anionic molybdenum amidato bisalkyl alkylidyne complex. *Journal of Organometallic Chemistry*, **2015**, 799-800, 223-225	2.3	4
29	Hydrogenation of small aromatic heterocycles at low temperatures. *Monthly Notices of the Royal Astronomical Society*, **2021**, 505, 3157-3164	4.3	4
28	Gas-phase spectroscopic characterization of neutral and ionic polycyclic aromatic phosphorus heterocycles (PAPHs). *Monthly Notices of the Royal Astronomical Society*, **2020**, 500, 2564-2576	4.3	3
27	Free energy reaction root mapping of alanine tripeptide in water. *Molecular Physics*, **2019**, 117, 2284-2292	2.7	3
26	Quantitative Distinction between Noble Metals Located in Mesopores from Those on the External Surface. *Chemistry - A European Journal*, **2021**, 27, 17012-17023	4.8	3
25	Predicting properties of periodic systems from cluster data: A case study of liquid water.. *Journal of Chemical Physics*, **2022**, 156, 114103	3.9	3
24	Copper coordination in formylglycine generating enzymes. *European Physical Journal: Special Topics* , **2019**, 227, 1657-1664	2.3	2
23	The role of atom tunneling in gas-phase reactions in planet-forming disks. *Astronomy and Astrophysics*, **2019**, 627, A45	5.1	2
22	Are different stoichiometries feasible for complexes between lymphotoxin-alpha and tumor necrosis factor receptor 1?. *BMC Structural Biology*, **2012**, 12, 8	2.7	2
21	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	5.1	2

20	Binding energies and sticking coefficients of H2 on crystalline and amorphous CO ice. *Astronomy and Astrophysics*, **2021**, 648, A84	5.1	2
19	Exploration of transferable and uniformly accurate neural network interatomic potentials using optimal experimental design. *Machine Learning: Science and Technology*, **2021**, 2, 035009	5.1	2
18	3D sub-nanometer analysis of glucose in an aqueous solution by cryo-atom probe tomography. *Scientific Reports*, **2021**, 11, 11607	4.9	2
17	Highly Active Cooperative Lewis Acid/Ammonium Salt Catalyst for the Enantioselective Hydroboration of Ketones. *Angewandte Chemie*, **2021**, 133, 5604-5613	3.6	2
16	Geometry Optimization in Internal Coordinates Based on Gaussian Process Regression: Comparison of Two Approaches. *Journal of Chemical Theory and Computation*, **2021**, 17, 5955-5967	6.4	2
15	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	6.4	2
14	Inside Cover: Hydrogen-Atom Tunneling Could Contribute to H2 Formation in Space (Angew. Chem. Int. Ed. 40/2010). *Angewandte Chemie - International Edition*, **2010**, 49, 7140-7140	16.4	1
13	Status and Direction of Atom Probe Analysis of Frozen Liquids.. *Microscopy and Microanalysis*, **2022**, 1-18	0.5	1
12	Reaction Mechanism of Ring-Closing Metathesis with a Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Catalyst. *Organometallics*, **2020**, 39, 3146-3159	3.8	1
11	HOCO formation in astrochemical environments by radical-induced H-abstraction from formic acid. *Monthly Notices of the Royal Astronomical Society*, **2019**, 482, 293-300	4.3	1
10	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	5.3	1
9	Neural-network assisted study of nitrogen atom dynamics on amorphous solid water II. Diffusion. *Monthly Notices of the Royal Astronomical Society*, **2022**, 510, 3063-3070	4.3	1
8	Thermally Averaged Magnetic Anisotropy Tensors via Machine Learning Based on Gaussian Moments. *Journal of Chemical Theory and Computation*, **2021**,	6.4	1
7	Asymmetric Hydroboration of Ketones by Cooperative Lewis Acid/Onium Salt Catalysis: A Quantum Chemical and Microkinetic Study to Combine Theory and Experiment. *ACS Catalysis*,1497-1507	13.1	0
6	Interplay of Polarity and Confinement in Asymmetric Catalysis with Chiral Rh Diene Complexes in Microemulsions. *Chemistry - A European Journal*, **2021**, 27, 16853-16870	4.8	0
5	Stable Cycling of Room-Temperature Sodium-Sulfur Batteries Based on an In Situ Crosslinked Gel Polymer Electrolyte. *Advanced Functional Materials*,2201191	15.6	0
4	Theoretische Chemie 2010. *Nachrichten Aus Der Chemie*, **2011**, 59, 284-290	0.1	
3	Innentitelbild: Tunneln von Wasserstoffatomen kann zur Bildung von H2 im Weltraum beitragen (Angew. Chem. 40/2010). *Angewandte Chemie*, **2010**, 122, 7296-7296	3.6	

2	Radiation chemistry in astrochemical models: From the laboratory to the ISM. *Proceedings of the International Astronomical Union*, **2019**, 15, 454-455	0.1
1	Ruthenium-Catalyzed Secondary Amine Formation Studied by Density Functional Theory. *ChemCatChem*, **2021**, 13, 1383-1388	5.2