# Johannes Kstner

## List of Publications by Year in Descending Order



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| 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 | Status and Direction of Atom Probe Analysis of Frozen Liquids.. *Microscopy and Microanalysis*, **2022**, 1-18 | 0.5 | 1 |
| 144 | Predicting properties of periodic systems from cluster data: A case study of liquid water.. *Journal of Chemical Physics*, **2022**, 156, 114103 | 3.9 | 3 |
| 143 | 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 |
| 142 | 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 |
| 141 | Carbon Atom Reactivity with Amorphous Solid Water: HO-Catalyzed Formation of HCO. *Journal of Physical Chemistry Letters*, **2021**, 12, 10854-10860 | 6.4 | 6 |
| 140 | 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 |
| 139 | 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 |
| 138 | Computational Study of the Hydrogenation Sequence of the Phosphorous Atom on Interstellar Dust Grains. *Astrophysical Journal*, **2021**, 910, 55 | 4.7 | 6 |
| 137 | Binding energies and sticking coefficients of H2 on crystalline and amorphous CO ice. *Astronomy and Astrophysics*, **2021**, 648, A84 | 5.1 | 2 |
| 136 | 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 |
| 135 | Hydrogenation of small aromatic heterocycles at low temperatures. *Monthly Notices of the Royal Astronomical Society*, **2021**, 505, 3157-3164 | 4.3 | 4 |
| 134 | 3D sub-nanometer analysis of glucose in an aqueous solution by cryo-atom probe tomography. *Scientific Reports*, **2021**, 11, 11607 | 4.9 | 2 |
| 133 | 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 |
| 132 | Ruthenium-Catalyzed Secondary Amine Formation Studied by Density Functional Theory. *ChemCatChem*, **2021**, 13, 1383-1388 | 5.2 | |
| 131 | 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 |
| 130 | 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 |
| 129 | Highly Active Cooperative Lewis Acid Ammonium Salt Catalyst for the Enantioselective Hydroboration of Ketones. *Angewandte Chemie*, **2021**, 133, 5604-5613 | 3.6 | 2 |

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| 128 | 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 |
| 127 | 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 |
| 126 | Interlayer Interactions as Design Tool for Large-Pore COFs. *Journal of the American Chemical Society*, **2021**, 143, 15711-15722 | 16.4 | 16 |
| 125 | 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 |
| 124 | Thermally Averaged Magnetic Anisotropy Tensors via Machine Learning Based on Gaussian Moments. *Journal of Chemical Theory and Computation*, **2021**, | 6.4 | 1 |
| 123 | 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 |
| 122 | A cryogenic ice setup to simulate carbon atom reactions in interstellar ices. *Review of Scientific Instruments*, **2020**, 91, 054501 | 1.7 | 12 |
| 121 | Comment on "Computational evidence for sulfur atom tunneling in the ring flipping reaction of S4N4" *Chemical Physics Letters*, **2020**, 754, 137678 | 2.5 | 6 |
| 120 | Adsorption of H on amorphous solid water studied with molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2020**, 22, 7552-7563 | 3.6 | 6 |
| 119 | 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 |
| 118 | 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 |
| 117 | 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 |
| 116 | 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 |
| 115 | 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 |
| 114 | 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 |
| 113 | Isomers in Interstellar Environments. I. The Case of Z- and E-cyanomethanimine. *Astrophysical Journal*, **2020**, 897, 158 | 4.7 | 9 |
| 112 | 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 |
| 111 | Reaction Mechanism of Ring-Closing Metathesis with a Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Catalyst. *Organometallics*, **2020**, 39, 3146-3159 | 3.8 | 1 |

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| 110 | 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 |
| 109 | Neural-network assisted study of nitrogen atom dynamics on amorphous solid water II. adsorption and desorption. *Monthly Notices of the Royal Astronomical Society*, **2020**, 499, 1373-1384 | 4.3 | 9 |
| 108 | Field evaporation and atom probe tomography of pure water tips. *Scientific Reports*, **2020**, 10, 20271 | 4.9 | 14 |
| 107 | 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 |
| 106 | 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 |
| 105 | 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 |
| 104 | Copper coordination in formylglycine generating enzymes. *European Physical Journal: Special Topics* , **2019**, 227, 1657-1664 | 2.3 | 2 |
| 103 | Formation of Acetaldehyde on CO-Rich Ices. *ACS Earth and Space Chemistry*, **2019**, 3, 958-963 | 3.2 | 18 |
| 102 | Unfolding of DNA by co-solutes: insights from Kirkwood–Buff integrals and transfer free energies. *European Physical Journal: Special Topics*, **2019**, 227, 1665-1679 | 2.3 | 16 |
| 101 | The role of atom tunneling in gas-phase reactions in planet-forming disks. *Astronomy and Astrophysics*, **2019**, 627, A45 | 5.1 | 2 |
| 100 | The Case of H2C3O Isomers, Revisited: Solving the Mystery of the Missing Propadienone. *Astrophysical Journal*, **2019**, 878, 80 | 4.7 | 19 |
| 99 | Gaussian Process Regression for Minimum Energy Path Optimization and Transition State Search. *Journal of Physical Chemistry A*, **2019**, 123, 9600-9611 | 2.8 | 14 |
| 98 | Molybdenum and Tungsten Alkylidyne Complexes Containing Mono-, Bi-, and Tridentate N-Heterocyclic Carbenes. *Organometallics*, **2019**, 38, 4133-4146 | 3.8 | 19 |
| 97 | 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 |
| 96 | Radiation chemistry in astrochemical models: From the laboratory to the ISM. *Proceedings of the International Astronomical Union*, **2019**, 15, 454-455 | 0.1 | |
| 95 | Silicate-mediated interstellar water formation: A theoretical study. *Monthly Notices of the Royal Astronomical Society*, **2019**, 482, 5389-5400 | 4.3 | 9 |
| 94 | Proton Affinities of N-Heterocyclic Olefins and Their Implications for Organocatalyst Design. *Journal of Organic Chemistry*, **2019**, 84, 2209-2218 | 4.2 | 25 |
| 93 | 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 | 4.8 | 12 |

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| 92 | Free energy reaction root mapping of alanine tripeptide in water. *Molecular Physics*, **2019**, 117, 2284-2292 | 2.7 | 3 |
| 91 | 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 |
| 90 | Gaussian process regression for geometry optimization. *Journal of Chemical Physics*, **2018**, 148, 094114 | 3.9 | 44 |
| 89 | Dual-Level Approach to Instanton Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 1865-1872 | 5.4 | 12 |
| 88 | Potential energy surface interpolation with neural networks for instanton rate calculations. *Journal of Chemical Physics*, **2018**, 148, 094106 | 3.9 | 14 |
| 87 | Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. *ChemCatChem*, **2018**, 10, 1052-1063 | 5.2 | 11 |
| 86 | The Lewis Pair Polymerization of Lactones Using Metal Halides and N-Heterocyclic Olefins: Theoretical Insights. *Molecules*, **2018**, 23, | 4.8 | 22 |
| 85 | Hydrogen transfer reactions of interstellar complex organic molecules. *Monthly Notices of the Royal Astronomical Society*, **2018**, 479, 2007-2015 | 4.3 | 26 |
| 84 | 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 |
| 83 | Calculation of Reaction Rate Constants in the Canonical and Microcanonical Ensemble. *Journal of Chemical Theory and Computation*, **2018**, 14, 5489-5498 | 6.4 | 11 |
| 82 | Gaussian Process Regression for Transition State Search. *Journal of Chemical Theory and Computation*, **2018**, 14, 5777-5786 | 6.4 | 28 |
| 81 | 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 |
| 80 | 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 |
| 79 | 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 |
| 78 | 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 |
| 77 | Asymmetric Ketone Reduction by Imine Reductases. *ChemBioChem*, **2017**, 18, 253-256 | 3.8 | 35 |
| 76 | On the Accessible Reaction Channels of Vinyl Gold(I) Species: and Pathways. *Chemistry - A European Journal*, **2017**, 23, 10901-10905 | 4.8 | 34 |
| 75 | 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 |

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| 74 | Rate constants from instanton theory via a microcanonical approach. *Journal of Chemical Physics*, **2017**, 146, 074105 | 3.9 | 21 |
| 73 | 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 |
| 72 | Importance of tunneling in H-abstraction reactions by OH radicals. *Astronomy and Astrophysics*, **2017**, 599, A132 | 5.1 | 12 |
| 71 | Influence of Surface and Bulk Water Ice on the Reactivity of a Water-forming Reaction. *Astrophysical Journal*, **2017**, 846, 43 | 4.7 | 22 |
| 70 | 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 |
| 69 | 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 |
| 68 | Atom Tunneling in the Water Formation Reaction H2 + OH -nH2O + H on an Ice Surface. *ACS Earth and Space Chemistry*, **2017**, 1, 399-410 | 3.2 | 29 |
| 67 | Instanton rate constant calculations close to and above the crossover temperature. *Journal of Computational Chemistry*, **2017**, 38, 2570-2580 | 3.5 | 21 |
| 66 | 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 |
| 65 | Tunneling Rate Constants for H2CO+H on Amorphous Solid Water Surfaces. *Astrophysical Journal*, **2017**, 850, 118 | 4.7 | 14 |
| 64 | Tunneling Reaction Kinetics for the Hydrogen Abstraction Reaction H + HS -nH + HS in the Interstellar Medium. *Journal of Physical Chemistry A*, **2017**, 121, 9736-9741 | 2.8 | 18 |
| 63 | 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 |
| 62 | Der Tunneleffekt von Atomen in der Chemie. *Angewandte Chemie*, **2016**, 128, 5488-5502 | 3.6 | 23 |
| 61 | QM/MM-Simulationen ergeben synergetische Substrat- und Sauerstoffaktivierung in Salicylat-Dioxygenase. *Angewandte Chemie*, **2016**, 128, 1182-1187 | 3.6 | 4 |
| 60 | Atom tunnelling in the reaction NH + H -nNH + H and its astrochemical relevance. *Faraday Discussions*, **2016**, 195, 69-80 | 3.6 | 13 |
| 59 | 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 |
| 58 | Gold(I) Vinylidene Complexes as Reactive Intermediates and Their Tendency to Backbond. *Chemistry - A European Journal*, **2016**, 22, 2892-5 | 4.8 | 57 |
| 57 | Synergistic Substrate and Oxygen Activation in Salicylate Dioxygenase Revealed by QM/MM Simulations. *Angewandte Chemie - International Edition*, **2016**, 55, 1168-72 | 16.4 | 27 |

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| 56 | Atom Tunneling in Chemistry. *Angewandte Chemie - International Edition*, **2016**, 55, 5400-13 | 16.4 | 124 |
| 55 | Reaction rates and kinetic isotope effects of H2 + OH -m H2O + H. *Journal of Chemical Physics*, **2016**, 144, 174303 | 3.9 | 23 |
| 54 | 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 |
| 53 | The Stabilizing Effects in Gold Carbene Complexes. *Angewandte Chemie - International Edition*, **2015**, 54, 10336-40 | 16.4 | 85 |
| 52 | Zu den stabilisierenden Effekten in Carbengoldkomplexen. *Angewandte Chemie*, **2015**, 127, 10477-10481 | 3.6 | 36 |
| 51 | N2 Binding to the FeMo-Cofactor of Nitrogenase. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2015**, 641, 118-122 | 1.3 | 26 |
| 50 | An anionic molybdenum amidato bisalkyl alkylidyne complex. *Journal of Organometallic Chemistry*, **2015**, 799-800, 223-225 | 2.3 | 4 |
| 49 | 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 |
| 48 | ChemShell□ modular software package for QM/MM simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 101-110 | 7.9 | 267 |
| 47 | 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 |
| 46 | Averaging techniques for reaction barriers in QM/MM simulations. *ChemPhysChem*, **2014**, 15, 3264-9 | 3.2 | 30 |
| 45 | Reaction mechanism of the bicopper enzyme peptidylglycine □hydroxylating monooxygenase. *Journal of Biological Chemistry*, **2014**, 289, 13726-38 | 5.4 | 25 |
| 44 | Nudged-elastic band used to find reaction coordinates based on the free energy. *Journal of Chemical Physics*, **2014**, 140, 074109 | 3.9 | 26 |
| 43 | Theory and simulation of atom tunneling in chemical reactions. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 158-168 | 7.9 | 67 |
| 42 | Tunneling above the crossover temperature. *Journal of Physical Chemistry A*, **2014**, 118, 78-82 | 2.8 | 27 |
| 41 | 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 |
| 40 | 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 |
| 39 | Path length determines the tunneling decay of substituted carbenes. *Chemistry - A European Journal*, **2013**, 19, 8207-12 | 4.8 | 34 |

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| 38 | A New Tabu-Search-Based Algorithm for Solvation of Proteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 814-21 | 6.4 | 11 |
| 37 | Reaction mechanism of monoamine oxidase from QM/MM calculations. *Journal of Physical Chemistry B*, **2013**, 117, 14238-46 | 3.4 | 52 |
| 36 | A Quadratically-Converging Nudged Elastic Band Optimizer. *Journal of Chemical Theory and Computation*, **2013**, 9, 3498-504 | 6.4 | 16 |
| 35 | Role of tunneling in the enzyme glutamate mutase. *Journal of Physical Chemistry B*, **2012**, 116, 13682-9 | 3.4 | 48 |
| 34 | Are different stoichiometries feasible for complexes between lymphotoxin-alpha and tumor necrosis factor receptor 1?. *BMC Structural Biology*, **2012**, 12, 8 | 2.7 | 2 |
| 33 | An algorithm to find minimum free-energy paths using umbrella integration. *Journal of Chemical Physics*, **2012**, 137, 034105 | 3.9 | 13 |
| 32 | Umbrella integration with higher-order correction terms. *Journal of Chemical Physics*, **2012**, 136, 234102 | 3.9 | 14 |
| 31 | Theoretische Chemie 2010. *Nachrichten Aus Der Chemie*, **2011**, 59, 284-290 | 0.1 | |
| 30 | Umbrella sampling. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 932-942 | 7.9 | 645 |
| 29 | Kinetic isotope effects calculated with the instanton method. *Journal of Computational Chemistry*, **2011**, 32, 3456-63 | 3.5 | 32 |
| 28 | 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 |
| 27 | Deuterium enrichment of interstellar methanol explained by atom tunneling. *Journal of Physical Chemistry A*, **2011**, 115, 10767-74 | 2.8 | 48 |
| 26 | Locating Instantons in Many Degrees of Freedom. *Journal of Chemical Theory and Computation*, **2011**, 7, 690-8 | 6.4 | 94 |
| 25 | Adaptive integration grids in instanton theory improve the numerical accuracy at low temperature. *Journal of Chemical Physics*, **2011**, 134, 184107 | 3.9 | 62 |
| 24 | 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 |
| 23 | The ribosome catalyzes peptide bond formation by providing high ionic strength. *Molecular Physics*, **2010**, 108, 293-306 | 1.7 | 17 |
| 22 | Tunneln von Wasserstoffatomen kann zur Bildung von H2 im Weltraum beitragen. *Angewandte Chemie*, **2010**, 122, 7508-7511 | 3.6 | 9 |
| 21 | Innentitelbild: Tunneln von Wasserstoffatomen kann zur Bildung von H2 im Weltraum beitragen (Angew. Chem. 40/2010). *Angewandte Chemie*, **2010**, 122, 7296-7296 | 3.6 | |

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| 20 | Hydrogen-atom tunneling could contribute to H2 formation in space. *Angewandte Chemie - International Edition*, **2010**, 49, 7350-2 | 16.4 | 64 |
| 19 | 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 |
| 18 | Umbrella integration in two or more reaction coordinates. *Journal of Chemical Physics*, **2009**, 131, 034109 | 3.9 | 45 |
| 17 | An embedded cluster study of the formation of water on interstellar dust grains. *Physical Chemistry Chemical Physics*, **2009**, 11, 5431-6 | 3.6 | 65 |
| 16 | Ectodomain orientation, conformational plasticity and oligomerization of ErbB1 receptors investigated by molecular dynamics. *Journal of Structural Biology*, **2009**, 167, 117-28 | 3.4 | 39 |
| 15 | DL-FIND: an open-source geometry optimizer for atomistic simulations. *Journal of Physical Chemistry A*, **2009**, 113, 11856-65 | 2.8 | 356 |
| 14 | Finite-temperature effects in enzymatic reactions Insights from QM/MM free-energy simulations. *Canadian Journal of Chemistry*, **2009**, 87, 1322-1337 | 0.9 | 57 |
| 13 | Superlinearly converging dimer method for transition state search. *Journal of Chemical Physics*, **2008**, 128, 014106 | 3.9 | 220 |
| 12 | 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 |
| 11 | 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 |
| 10 | Analysis of the statistical error in umbrella sampling simulations by umbrella integration. *Journal of Chemical Physics*, **2006**, 124, 234106 | 3.9 | 132 |
| 9 | 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 |
| 8 | Model for acetylene reduction by nitrogenase derived from density functional theory. *Inorganic Chemistry*, **2005**, 44, 4568-75 | 5.1 | 29 |
| 7 | 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 |
| 6 | Towards an understanding of the workings of nitrogenase from DFT calculations. *ChemPhysChem*, **2005**, 6, 1724-6 | 3.2 | 36 |
| 5 | Activation and protonation of dinitrogen at the FeMo cofactor of nitrogenase. *Journal of Chemical Physics*, **2005**, 123, 074306 | 3.9 | 39 |
| 4 | Projector augmented wave method:ab initio molecular dynamics with full wave functions. *Bulletin of Materials Science*, **2003**, 26, 33-41 | 1.7 | 274 |
| 3 | Nitrogen binding to the FeMo-cofactor of nitrogenase. *Journal of the American Chemical Society*, **2003**, 125, 15772-8 | 16.4 | 102 |

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| 2 | 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 |
| 1 | Stable Cycling of Room-Temperature Sodium-Sulfur Batteries Based on an In Situ Crosslinked Gel Polymer Electrolyte. *Advanced Functional Materials*,2201191 | 15.6 | 0 |