Hannes Jnsson

List of Publications by Citations

234 papers	45,504 citations	57 h-index	213 g-index
247 ext. papers	52,385 ext. citations	4.2 avg, IF	7.69 L-index

#	Paper	IF	Citations
234	A climbing image nudged elastic band method for finding saddle points and minimum energy paths. *Journal of Chemical Physics*, **2000**, 113, 9901-9904	3.9	11184
233	A fast and robust algorithm for Bader decomposition of charge density. *Computational Materials Science*, **2006**, 36, 354-360	3.2	5896
232	Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. *Journal of Physical Chemistry B*, **2004**, 108, 17886-17892	3.4	5882
231	Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points. *Journal of Chemical Physics*, **2000**, 113, 9978-9985	3.9	5577
230	A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives. *Journal of Chemical Physics*, **1999**, 111, 7010-7022	3.9	1971
229	Reversible work transition state theory: application to dissociative adsorption of hydrogen. *Surface Science*, **1995**, 324, 305-337	1.8	1699
228	Nudged elastic band method for finding minimum energy paths of transitions **1998**,		921
227	Systematic analysis of local atomic structure combined with 3D computer graphics. *Computational Materials Science*, **1994**, 2, 279-286	3.2	833
226	A theoretical evaluation of possible transition metal electro-catalysts for N2 reduction. *Physical Chemistry Chemical Physics*, **2012**, 14, 1235-45	3.6	810
225	Modeling the Electrochemical Hydrogen Oxidation and Evolution Reactions on the Basis of Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 18182-18197	3.8	743
224	Quantum and thermal effects in H2 dissociative adsorption: Evaluation of free energy barriers in multidimensional quantum systems. *Physical Review Letters*, **1994**, 72, 1124-1127	7.4	669
223	Density functional theory calculations for the hydrogen evolution reaction in an electrochemical double layer on the Pt(111) electrode. *Physical Chemistry Chemical Physics*, **2007**, 9, 3241-50	3.6	533
222	Icosahedral ordering in the Lennard-Jones liquid and glass. *Physical Review Letters*, **1988**, 60, 2295-2298	7.4	474
221	Comparison of methods for finding saddle points without knowledge of the final states. *Journal of Chemical Physics*, **2004**, 121, 9776-92	3.9	388
220	Long time scale kinetic Monte Carlo simulations without lattice approximation and predefined event table. *Journal of Chemical Physics*, **2001**, 115, 9657-9666	3.9	358
219	Structural changes accompanying densification of random hard-sphere packings. *Physical Review E*, **1993**, 47, 3975-3984	2.4	323
218	Global transition path search for dislocation formation in Ge on Si(001). *Computer Physics Communications*, **2016**, 205, 13-21	4.2	203

217	NWChem: Past, present, and future. *Journal of Chemical Physics*, **2020**, 152, 184102	3.9	187
216	Improved initial guess for minimum energy path calculations. *Journal of Chemical Physics*, **2014**, 140, 214106	3.9	184
215	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 49-70	3.6	171
214	Predicting catalysis: understanding ammonia synthesis from first-principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 17719-35	3.4	168
213	Molecular multipole moments of water molecules in ice Ih. *Journal of Chemical Physics*, **1998**, 109, 4546-4551	3.9	159
212	Theoretical calculations of CH4 and H2 associative desorption from Ni(111): could subsurface hydrogen play an important role?. *Journal of Chemical Physics*, **2006**, 124, 044706	3.9	146
211	Calculations of Product Selectivity in Electrochemical CO2 Reduction. *ACS Catalysis*, **2018**, 8, 5240-5249	13.1	135
210	Comparison of quantum dynamics and quantum transition state theory estimates of the H + CH4 reaction rate. *Journal of Physical Chemistry A*, **2009**, 113, 4468-78	2.8	127
209	Theoretical calculations of dissociative adsorption of CH4 on an Ir(111) surface. *Physical Review Letters*, **2001**, 86, 664-7	7.4	124
208	First-principles Green's-function method for surface calculations: A pseudopotential localized basis set approach. *Physical Review B*, **2017**, 96,	3.3	122
207	Diffusion mechanisms relevant to metal crystal growth: Pt/Pt(111). *Surface Science*, **1994**, 317, 15-36	1.8	119
206	Silica glass structure generation for ab initio calculations using small samples of amorphous silica. *Physical Review B*, **2005**, 71,	3.3	118
205	Theoretical studies of atomic-scale processes relevant to crystal growth. *Annual Review of Physical Chemistry*, **2000**, 51, 623-53	15.7	116
204	Investigation of the reliability of density functional methods: Reaction and activation energies for Si–Si bond cleavage and H2 elimination from silanes. *Journal of Chemical Physics*, **1996**, 104, 148-158	3.9	107
203	Method for finding mechanism and activation energy of magnetic transitions, applied to skyrmion and antivortex annihilation. *Computer Physics Communications*, **2015**, 196, 335-347	4.2	98
202	Generalized path integral based quantum transition state theory. *Chemical Physics Letters*, **1997**, 278, 91-96	2.5	98
201	Experimental and Theoretical Study of the Rotation of Si Ad-dimers on the Si(100) Surface. *Physical Review Letters*, **1996**, 77, 2518-2521	7.4	97
200	Multidimensional reactive transport modeling of CO2 mineral sequestration in basalts at the Hellisheidi geothermal field, Iceland. *International Journal of Greenhouse Gas Control*, **2012**, 9, 24-40	4.2	95

199	Multipole moments of water molecules in clusters and ice Ih from first principles calculations. *Journal of Chemical Physics*, **1999**, 111, 6011-6015	3.9	95
198	Atomistic Determination of Cross-Slip Pathway and Energetics. *Physical Review Letters*, **1997**, 79, 3676-3679	7.4	91
197	Simulation of surface processes. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 944-9	11.5	90
196	Lifetime of racetrack skyrmions. *Scientific Reports*, **2018**, 8, 3433	4.9	88
195	Small Pd Clusters, up to the tetramer at least, are highly mobile on the MgO(100) surface. *Physical Review Letters*, **2005**, 95, 146103	7.4	84
194	Methods for Finding Saddle Points and Minimum Energy Paths **2002**, 269-302		84
193	Nudged elastic band calculations accelerated with Gaussian process regression. *Journal of Chemical Physics*, **2017**, 147, 152720	3.9	79
192	Thermal Diffusion Processes in Metal-Tip-Surface Interactions: Contact Formation and Adatom Mobility. *Physical Review Letters*, **1996**, 77, 5067-5070	7.4	79
191	Multiple time scale simulations of metal crystal growth reveal the importance of multiatom surface processes. *Physical Review Letters*, **2003**, 90, 116101	7.4	78
190	Magic-number gold nanoclusters with diameters from 1 to 3.5 nm: relative stability and catalytic activity for CO oxidation. *Nano Letters*, **2015**, 15, 682-8	11.5	76
189	The effect of the Perdew-Zunger self-interaction correction to density functionals on the energetics of small molecules. *Journal of Chemical Physics*, **2012**, 137, 124102	3.9	75
188	Diffusion of Ge below the Si(100) surface: theory and experiment. *Physical Review Letters*, **2000**, 84, 2441-4	7.4	70
187	Simulations of hydrogen diffusion at grain boundaries in aluminum. *Acta Materialia*, **2009**, 57, 4036-4045	8.4	69
186	Si adatom binding and diffusion on the Si(100) surface: Comparison of ab initio, semiempirical and empirical potential results. *Journal of Chemical Physics*, **1995**, 102, 1044-1056	3.9	69
185	Importance of complex orbitals in calculating the self-interaction-corrected ground state of atoms. *Physical Review A*, **2011**, 84,	2.6	67
184	Pd diffusion on MgO(100): The role of defects and small cluster mobility. *Surface Science*, **2006**, 600, 1351-1362	1.8	66
183	Reversible work based quantum transition state theory. *Journal of Chemical Physics*, **1994**, 101, 8964-8973	3.9	64
182	Mechanism and activation energy of magnetic skyrmion annihilation obtained from minimum energy path calculations. *Physical Review B*, **2016**, 94,	3.3	63

181	Atomic structure of □SiC(100) surfaces: an ab initio study. *Surface Science*, **1995**, 330, 265-275	1.8	63
180	Excess energy of grain-boundary trijunctions: an atomistic simulation study. *Acta Materialia*, **1999**, 47, 2821-2829	8.4	61
179	Variational, Self-Consistent Implementation of the Perdew-Zunger Self-Interaction Correction with Complex Optimal Orbitals. *Journal of Chemical Theory and Computation*, **2014**, 10, 5324-37	6.4	59
178	Hydrogen adsorption and desorption at the Pt(110)-(1□) surface: experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2013**, 15, 6323-32	3.6	59
177	Unitary Optimization of Localized Molecular Orbitals. *Journal of Chemical Theory and Computation*, **2013**, 9, 5365-72	6.4	56
176	Adsorption of water monomer and clusters on platinum(111) terrace and related steps and kinks. *Surface Science*, **2010**, 604, 1978-1986	1.8	52
175	Electric fields in ice and near water clusters. *Journal of Chemical Physics*, **2000**, 112, 3285-3292	3.9	51
174	Diffusion and Island formation on the ice Ih basal plane surface. *Computational Materials Science*, **2001**, 20, 325-336	3.2	50
173	Two- and three-body forces in the interaction of He atoms with Xe overlayers adsorbed on (0001) graphite. *Journal of Chemical Physics*, **1989**, 91, 6477-6493	3.9	50
172	Pipek-Mezey Orbital Localization Using Various Partial Charge Estimates. *Journal of Chemical Theory and Computation*, **2014**, 10, 642-9	6.4	49
171	EON: software for long time simulations of atomic scale systems. *Modelling and Simulation in Materials Science and Engineering*, **2014**, 22, 055002	2	49
170	Structure and molecular properties of adsorbates at low coverage: Light-atom scattering from adsorbed Xe and CO. *Physical Review B*, **1984**, 30, 2241-2244	3.3	49
169	Low-temperature homoepitaxial growth of Pt(111) in simulated vapor deposition. *Physical Review B* , **1994**, 49, 2208-2211	3.3	48
168	Assessment of Constant-Potential Implicit Solvation Calculations of Electrochemical Energy Barriers for H2 Evolution on Pt. *Journal of Physical Chemistry C*, **2019**, 123, 4116-4124	3.8	47
167	Harmonic transition-state theory of thermal spin transitions. *Physical Review B*, **2012**, 85,	3.3	46
166	Combined experimental and theoretical study on the nature and the metastable decay pathways of the amino acid ion fragment [M-H]-. *Angewandte Chemie - International Edition*, **2007**, 46, 8057-9	16.4	46
165	What determines the sticking probability of water molecules on ice?. *Physical Review Letters*, **2005**, 95, 223201	7.4	44
164	Dimer and String Formation during Low Temperature Silicon Deposition on Si(100). *Physical Review Letters*, **1996**, 77, 1326-1329	7.4	44

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162	Parallel implementation of -point pseudopotential plane-wave DFT with exact exchange. *Journal of Computational Chemistry*, **2011**, 32, 54-69	3.5	42
161	Optimization of hyperplanar transition states. *Journal of Chemical Physics*, **2001**, 115, 9644-9656	3.9	42
160	Theoretical study of kinks on screw dislocation in silicon. *Physical Review B*, **2008**, 77,	3.3	41
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158	Spirit: Multifunctional framework for atomistic spin simulations. *Physical Review B*, **2019**, 99,	3.3	38
157	Faraday efficiency and mechanism of electrochemical surface reactions: CO reduction and H formation on Pt(111). *Faraday Discussions*, **2016**, 195, 619-636	3.6	37
156	Kinetic Monte Carlo simulations of Pd deposition and island growth on MgO(100). *Surface Science*, **2007**, 601, 3133-3142	1.8	35
155	Migration of O vacancies in -quartz: The effect of excitons and electron holes. *Physical Review B*, **2001**, 64,	3.3	35
154	Development and evaluation of a thermodynamic dataset for phases of interest in CO2 mineral sequestration in basaltic rocks. *Chemical Geology*, **2012**, 304-305, 26-38	4.2	33
153	Local density of states analysis using Bader decomposition for N2 and CO2 adsorbed on Pt(110)-(1 2) electrodes. *Journal of Chemical Physics*, **2012**, 137, 164705	3.9	32
152	Atomic structure of -SiC(100) surfaces: a study using the Tersoff potential. *Surface Science*, **1994**, 316, 181-188	1.8	32
151	Hydrogen atom scattering from physisorbed overlayers. *Surface Science*, **1985**, 155, 499-534	1.8	32
150	An ab initio study of self-trapped excitons in -quartz. *Journal of Chemical Physics*, **2003**, 118, 6582-6593	3.9	31
149	Nudged Elastic Band Calculations Accelerated with Gaussian Process Regression Based on Inverse Interatomic Distances. *Journal of Chemical Theory and Computation*, **2019**, 15, 6738-6751	6.4	29
148	A transferable H2O interaction potential based on a single center multipole expansion: SCME. *Physical Chemistry Chemical Physics*, **2013**, 15, 16542-56	3.6	29
147	Self-interaction corrected density functional calculations of molecular Rydberg states. *Journal of Chemical Physics*, **2013**, 139, 194102	3.9	29
146	Adsorption of water dimer on platinum(111): identification of the -OH Pt hydrogen bond. *ACS Nano*, **2014**, 8, 11583-90	16.7	28

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144	Ultrafast structural dynamics in Rydberg excited N,N,N?,N?-tetramethylethylenediamine: conformation dependent electron lone pair interaction and charge delocalization. *Chemical Science*, **2014**, 5, 4394-4403	9.4	27
143	Charge localization in a diamine cation provides a test of energy functionals and self-interaction correction. *Nature Communications*, **2016**, 7, 11013	17.4	27
142	Optimal atomic structure of amorphous silicon obtained from density functional theory calculations. *New Journal of Physics*, **2017**, 19, 063018	2.9	26
141	Size and shape dependence of thermal spin transitions in nanoislands. *Physical Review Letters*, **2013** , 110, 020604	7.4	26
140	Absorption and Resonance Raman Study of the2B1(X)⁄A2(A) Transition of Chlorine Dioxide in the Gas Phase. *Journal of Physical Chemistry A*, **1999**, 103, 1748-1757	2.8	26
139	Theory and Applications of Generalized Pipek-Mezey Wannier Functions. *Journal of Chemical Theory and Computation*, **2017**, 13, 460-474	6.4	25
138	Energy surface and lifetime of magnetic skyrmions. *Journal of Magnetism and Magnetic Materials*, **2018**, 459, 236-240	2.8	25
137	Atomic exchange processes in sputter deposition of Pt on Pt(111). *Surface Science*, **1995**, 324, 35-46	1.8	25
136	Variational Density Functional Calculations of Excited States via Direct Optimization. *Journal of Chemical Theory and Computation*, **2020**, 16, 6968-6982	6.4	25
135	Duplication, Collapse, and Escape of Magnetic Skyrmions Revealed Using a Systematic Saddle Point Search Method. *Physical Review Letters*, **2018**, 121, 197202	7.4	25
134	Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex. *Journal of Chemical Theory and Computation*, **2017**, 13, 6010-6022	6.4	24
133	The effect of confinement and defects on the thermal stability of skyrmions. *Physica B: Condensed Matter*, **2018**, 549, 6-9	2.8	24
132	Dynamics of basaltic glass dissolution Capturing microscopic effects in continuum scale models. *Geochimica Et Cosmochimica Acta*, **2013**, 121, 311-327	5.5	24
131	Finding possible transition states of defects in silicon-carbide and alpha-iron using the dimer method. *Nuclear Instruments & Methods in Physics Research B*, **2003**, 202, 1-7	1.2	24
130	Calculations of Al dopant in quartz using a variational implementation of the Perdew⁄unger self-interaction correction. *New Journal of Physics*, **2015**, 17, 083006	2.9	23
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128	Computational Study of Electrochemical CO 2 Reduction at Transition Metal Electrodes. *Procedia Computer Science*, **2015**, 51, 1865-1871	1.6	23

127	Calculations of dislocation mobility using Nudged Elastic Band method and first principles DFT calculations. *Philosophical Magazine*, **2008**, 88, 91-100	1.6	23
126	Efficient Sampling of Saddle Points with the Minimum-Mode Following Method. *SIAM Journal of Scientific Computing*, **2011**, 33, 633-652	2.6	22
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122	Long-timescale simulations of diffusion in molecular solids. *Physical Chemistry Chemical Physics*, **2012**, 14, 10844-52	3.6	21
121	The effect of coadsorbed water on the stability, configuration and interconversion of formyl (HCO) and hydroxymethylidyne (COH) on platinum (111). *Chemical Physics Letters*, **2012**, 541, 32-38	2.5	21
120	On the laterally averaged interaction potential between He atoms and the (0001) surface of graphite. *Chemical Physics Letters*, **1986**, 129, 139-143	2.5	21
119	Efficient evaluation of atom tunneling combined with electronic structure calculations. *Journal of Chemical Physics*, **2018**, 148, 102334	3.9	20
118	Self-interaction corrected density functional calculations of Rydberg states of molecular clusters: N,N-dimethylisopropylamine. *Journal of Chemical Physics*, **2014**, 141, 234308	3.9	20
117	Long time scale simulation of a grain boundary in copper. *New Journal of Physics*, **2009**, 11, 073034	2.9	20
116	Elastic sheet method for identifying atoms in molecules. *Journal of Chemical Physics*, **1999**, 111, 10664-10669	3.6	20
115	Variational calculations of excited states direct optimization of the orbitals in DFT. *Faraday Discussions*, **2020**, 224, 448-466	3.6	19
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111	Molecular dynamics simulations of a pressure-induced glass transition. *Journal of Chemical Physics*, **1995**, 102, 1796-1805	3.9	19
110	A parallel implementation of the Car-Parrinello method by orbital decomposition. *Computer Physics Communications*, **1994**, 81, 1-18	4.2	19

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107	Experimental and theoretical study of the metastable decay of negatively charged nucleosides in the gas phase. *Physical Chemistry Chemical Physics*, **2011**, 13, 15283-90	3.6	18
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105	An embedded atom method potential for the h.c.p. metal Zr. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1995**, 71, 1041-1056		18
104	Atom scattering as a quantitative surface probe: Noble-gas monolayer and bilayer adsorbed on graphite. *Physical Review B*, **1984**, 30, 4203-4206	3.3	18
103	Path Optimization with Application to Tunneling. *Lecture Notes in Computer Science*, **2012**, 45-55	0.9	18
102	Reassignment of 'magic numbers' for Au clusters of decahedral and FCC structural motifs. *Nanoscale*, **2018**, 10, 5124-5132	7.7	17
101	Molecular reordering processes on ice (0001) surfaces from long timescale simulations. *Journal of Chemical Physics*, **2014**, 141, 234706	3.9	17
100	Simulated Annealing with Coarse Graining and Distributed Computing. *Lecture Notes in Computer Science*, **2012**, 34-44	0.9	17
99	Distributed implementation of the adaptive kinetic Monte Carlo method. *Mathematics and Computers in Simulation*, **2010**, 80, 1487-1498	3.3	17
98	Cleavage and recovery of molecular water in silica. *Journal of Physical Chemistry B*, **2005**, 109, 10936-45	3.4	17
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96	Minimum energy path calculations with Gaussian process regression. *Nanosystems: Physics, Chemistry, Mathematics*, **2016**, 925-935	1.8	17
95	Determination of the structure and properties of an edge dislocation in rutile TiO2. *Acta Materialia*, **2019**, 163, 199-207	8.4	17
94	Observation of Structural Wavepacket Motion: The Umbrella Mode in Rydberg-Excited N-Methyl Morpholine. *Journal of Physical Chemistry Letters*, **2017**, 8, 3740-3744	6.4	16
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90	Simulations of the Oxidation and Degradation of Platinum Electrocatalysts. *Small*, **2020**, 16, e1905159	11	16
89	On the interplay of solvent and conformational effects in simulated excited-state dynamics of a copper phenanthroline photosensitizer. *Physical Chemistry Chemical Physics*, **2020**, 22, 748-757	3.6	16
88	Removing External Degrees of Freedom from Transition-State Search Methods using Quaternions. *Journal of Chemical Theory and Computation*, **2015**, 11, 1055-62	6.4	15
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78	RAW quantum transition state theory **1998**,		13
77	Finding mechanism of transitions in complex systems: formation and migration of dislocation kinks in a silicon crystal. *Journal of Physics Condensed Matter*, **2009**, 21, 084210	1.8	12
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75	R-NEB: Accelerated Nudged Elastic Band Calculations by Use of Reflection Symmetry. *Journal of Chemical Theory and Computation*, **2019**, 15, 3215-3222	6.4	11
74	Effect of hydrogen adsorption on the magnetic properties of a surface nanocluster of iron. *Physical Review B*, **2013**, 88,	3.3	11

73	Atomic Scale Formation Mechanism of Edge Dislocation Relieving Lattice Strain in a GeSi overlayer on Si(001). *Scientific Reports*, **2017**, 7, 11966	4.9	11
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70	Minimum Mode Saddle Point Searches Using Gaussian Process Regression with Inverse-Distance Covariance Function. *Journal of Chemical Theory and Computation*, **2020**, 16, 499-509	6.4	11
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67	Towards an Optimal Gradient-dependent Energy Functional of the PZ-SIC Form. *Procedia Computer Science*, **2015**, 51, 1858-1864	1.6	9
66	A method for finding the ridge between saddle points applied to rare event rate estimates. *Physical Chemistry Chemical Physics*, **2012**, 14, 2884-91	3.6	9
65	Potential Energy Surfaces and Rates of Spin Transitions. *Zeitschrift Fur Physikalische Chemie*, **2013**, 1307080003[illegible]10008	[illegible]	9
64	Optimization of hyperplanar transition states: Application to 2D test problems. *Computer Physics Communications*, **2005**, 169, 284-288	4.2	9
63	Optimization of Functionals of Orthonormal Functions in the Absence of Unitary Invariance. *Lecture Notes in Computer Science*, **2012**, 23-33	0.9	9
62	Self-Interaction Corrected Functional Calculations of a Dipole-Bound Molecular Anion. *Journal of Physical Chemistry Letters*, **2016**, 7, 2068-73	6.4	9
61	Effect of Magnetic States on the Reactivity of an FCC(111) Iron Surface. *Journal of Physical Chemistry C*, **2014**, 118, 15863-15873	3.8	8
60	Magnetic exchange force microscopy: theoretical analysis of induced magnetization reversals. *Nanoscale*, **2017**, 9, 13320-13325	7.7	8
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58	Elucidation of temperature-programmed desorption of high-coverage hydrogen on Pt(211), Pt(221), Pt(533) and Pt(553) based on density functional theory calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 17142-17151	3.6	7
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56	Truncated minimum energy path method for finding first order saddle points. *Nanosystems: Physics, Chemistry, Mathematics*, **2017**, 586-595	1.8	7

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54	Transition state theory approach to polymer escape from a one dimensional potential well. *Journal of Chemical Physics*, **2015**, 142, 224906	3.9	6
53	Efficient optimization method for finding minimum energy paths of magnetic transitions. *Journal of Physics Condensed Matter*, **2020**, 32, 345901	1.8	6
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51	Polarizable Embedding with a Transferable HO Potential Function I: Formulation and Tests on Dimer. *Journal of Chemical Theory and Computation*, **2019**, 15, 6562-6577	6.4	6
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