Hannes Jnsson

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Lifetime of skyrmions in discrete systems with infinitesimal lattice constant. *Journal of Magnetism and Magnetic Materials*, **2022**, 549, 168974	2.8	0
233	Mechanism of Interlayer Transport on a Growing Au(111) Surface: 2D vs. 3D Growth. *Surfaces and Interfaces*, **2022**, 101944	4.1	0
232	Variational Density Functional Calculations of Excited States: Conical Intersection and Avoided Crossing in Ethylene Bond Twisting.. *Journal of Physical Chemistry Letters*, **2022**, 3990-3999	6.4	2
231	Observation of Electric-Field-Induced Liberation of Guest Molecules from Clathrate Hydrate. *Journal of Physical Chemistry Letters*, **2021**, 12, 10410-10416	6.4	0
230	Mn Dimer Can Be Described Accurately with Density Functional Calculations When Self-Interaction Correction Is Applied. *Journal of Physical Chemistry Letters*, **2021**, 12, 4240-4246	6.4	4
229	Competing HCOOH and CO Pathways in CO2 Electroreduction at Copper Electrodes: Calculations of Voltage-Dependent Activation Energy. *Journal of Physical Chemistry C*, **2021**, 125, 13802-13808	3.8	2
228	Method for Calculating Excited Electronic States Using Density Functionals and Direct Orbital Optimization with Real Space Grid or Plane-Wave Basis Set. *Journal of Chemical Theory and Computation*, **2021**, 17, 5034-5049	6.4	5
227	Nudged Elastic Band Method for Molecular Reactions Using Energy-Weighted Springs Combined with Eigenvector Following. *Journal of Chemical Theory and Computation*, **2021**, 17, 4929-4945	6.4	22
226	Fast and robust algorithm for energy minimization of spin systems applied in an analysis of high temperature spin configurations in terms of skyrmion density. *Computer Physics Communications*, **2021**, 260, 107749	4.2	5
225	Localized and Delocalized States of a Diamine Cation: Resolution of a Controversy. *Journal of Physical Chemistry Letters*, **2021**, 12, 1250-1255	6.4	1
224	Elastic Collision Based Dynamic Partitioning Scheme for Hybrid Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 5863-5875	6.4	2
223	Assessment of the Accuracy of Density Functionals for Calculating Oxygen Reduction Reaction on Nitrogen-Doped Graphene. *Journal of Chemical Theory and Computation*, **2021**, 17, 6405-6415	6.4	1
222	Direct energy minimization based on exponential transformation in density functional calculations of finite and extended systems. *Computer Physics Communications*, **2021**, 267, 108047	4.2	2
221	Efficient optimization method for finding minimum energy paths of magnetic transitions. *Journal of Physics Condensed Matter*, **2020**, 32, 345901	1.8	6
220	Coupled quasimonopoles in chiral magnets. *Physical Review B*, **2020**, 101,	3.3	10
219	NWChem: Past, present, and future. *Journal of Chemical Physics*, **2020**, 152, 184102	3.9	187
218	Variational calculations of excited states direct optimization of the orbitals in DFT. *Faraday Discussions*, **2020**, 224, 448-466	3.6	19

217	Skyrmions in antiferromagnets: Thermal stability and the effect of external field and impurities. *Journal of Applied Physics*, **2020**, 127, 213906	2.5	6
216	Magnetic skyrmion annihilation by quantum mechanical tunneling. *New Journal of Physics*, **2020**, 22, 083013	2.5	3
215	Cuboctahedral Platinum Nanoparticles: Simulations of the Oxidation and Degradation of Platinum Electrocatalysts (Small 5/2020). *Small*, **2020**, 16, 2070027	11	1
214	Atomic and electronic structures of a vacancy in amorphous silicon. *Physical Review B*, **2020**, 101,	3.3	1
213	Fully self-consistent calculations of magnetic structure within non-collinear Alexander-Anderson model. *Nanosystems: Physics, Chemistry, Mathematics*, **2020**, 11, 65-77	1.8	2
212	Exploring Potential Energy Surfaces with Saddle Point Searches **2020**, 689-714		2
211	Simulations of the Oxidation and Degradation of Platinum Electrocatalysts. *Small*, **2020**, 16, e1905159	11	16
210	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
209	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
208	Variational Density Functional Calculations of Excited States via Direct Optimization. *Journal of Chemical Theory and Computation*, **2020**, 16, 6968-6982	6.4	25
207	Stability of long-lived antiskyrmions in the Mn-Pt-Sn tetragonal Heusler material. *Physical Review B*, **2020**, 102,	3.3	4
206	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
205	Density functional theory calculations and thermodynamic analysis of bridgmanite surface structure. *Physical Chemistry Chemical Physics*, **2019**, 21, 1009-1013	3.6	3
204	Spirit: Multifunctional framework for atomistic spin simulations. *Physical Review B*, **2019**, 99,	3.3	38
203	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
202	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
201	Addition to "Assessment of Constant-Potential Implicit Solvation Calculations of Electrochemical Energy Barriers for H2 Evolution on Pt" *Journal of Physical Chemistry C*, **2019**, 123, 15875-15875	3.8	5
200	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

199	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
198	Polarizable Embedding with a Transferable HO Potential Function II: Application to (HO) Clusters and Liquid Water. *Journal of Chemical Theory and Computation*, **2019**, 15, 6578-6587	6.4	5
197	Effect of H adsorption on the magnetic properties of an Fe island on a W(110) surface. *Physical Review B*, **2019**, 100,	3.3	1
196	Determination of the structure and properties of an edge dislocation in rutile TiO2. *Acta Materialia*, **2019**, 163, 199-207	8.4	17
195	Density Functional Theory Calculations and Thermodynamic Analysis of the Forsterite Mg2SiO4(010) Surface. *Journal of Physical Chemistry C*, **2019**, 123, 464-472	3.8	7
194	Reassignment of 'magic numbers' for Au clusters of decahedral and FCC structural motifs. *Nanoscale*, **2018**, 10, 5124-5132	7.7	17
193	Lifetime of racetrack skyrmions. *Scientific Reports*, **2018**, 8, 3433	4.9	88
192	Calculations of Product Selectivity in Electrochemical CO2 Reduction. *ACS Catalysis*, **2018**, 8, 5240-5249	13.1	135
191	Efficient evaluation of atom tunneling combined with electronic structure calculations. *Journal of Chemical Physics*, **2018**, 148, 102334	3.9	20
190	Energy surface and lifetime of magnetic skyrmions. *Journal of Magnetism and Magnetic Materials*, **2018**, 459, 236-240	2.8	25
189	The effect of confinement and defects on the thermal stability of skyrmions. *Physica B: Condensed Matter*, **2018**, 549, 6-9	2.8	24
188	Duplication, Collapse, and Escape of Magnetic Skyrmions Revealed Using a Systematic Saddle Point Search Method. *Physical Review Letters*, **2018**, 121, 197202	7.4	25
187	Reply to: "The diamine cation is not a chemical example where density functional theory fails". *Nature Communications*, **2018**, 9, 5348	17.4	3
186	Exploring Potential Energy Surfaces with Saddle Point Searches **2018**, 1-26		1
185	Atomic scale simulations of heterogeneous electrocatalysis: recent advances. *Advances in Physics: X* , **2017**, 2, 481-495	5.1	14
184	Optimal atomic structure of amorphous silicon obtained from density functional theory calculations. *New Journal of Physics*, **2017**, 19, 063018	2.9	26
183	Theory and Applications of Generalized Pipek-Mezey Wannier Functions. *Journal of Chemical Theory and Computation*, **2017**, 13, 460-474	6.4	25
182	Long-Time Scale Simulations of Tunneling-Assisted Diffusion of Hydrogen on Ice Surfaces at Low Temperature. *Journal of Physical Chemistry C*, **2017**, 121, 1648-1657	3.8	13

181	Improved Minimum Mode Following Method for Finding First Order Saddle Points. *Journal of Chemical Theory and Computation*, **2017**, 13, 125-134	6.4	18
180	Nudged elastic band calculations accelerated with Gaussian process regression. *Journal of Chemical Physics*, **2017**, 147, 152720	3.9	79
179	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
178	Ultrafast X-ray absorption study of longitudinal-transverse phonon coupling in electrolyte aqueous solution. *Physical Chemistry Chemical Physics*, **2017**, 19, 27266-27274	3.6	1
177	Coherence in nonradiative transitions: internal conversion in Rydberg-excited N-methyl and N-ethyl morpholine. *Physical Chemistry Chemical Physics*, **2017**, 19, 26403-26411	3.6	19
176	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
175	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
174	Magnetic exchange force microscopy: theoretical analysis of induced magnetization reversals. *Nanoscale*, **2017**, 9, 13320-13325	7.7	8
173	First-principles Green's-function method for surface calculations: A pseudopotential localized basis set approach. *Physical Review B*, **2017**, 96,	3.3	122
172	Energy surface and transition rates in a hexagonal element of spin ice. *Journal of Physics: Conference Series*, **2017**, 903, 012006	0.3	
171	The effect of temperature and external field on transitions in elements of kagome spin ice. *New Journal of Physics*, **2017**, 19, 113008	2.9	7
170	Calculations of the onset temperature for tunneling in multispin systems. *Nanosystems: Physics, Chemistry, Mathematics*, **2017**, 454-461	1.8	2
169	Truncated minimum energy path method for finding first order saddle points. *Nanosystems: Physics, Chemistry, Mathematics*, **2017**, 586-595	1.8	7
168	Instantons describing tunneling between magnetic states at finite temperature. *Nanosystems: Physics, Chemistry, Mathematics*, **2017**, 746-759	1.8	2
167	Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdew-Zunger Self-Interaction Correction to Density Functional Theory. *Journal of Chemical Theory and Computation*, **2016**, 12, 4296-302	6.4	23
166	Mechanism and activation energy of magnetic skyrmion annihilation obtained from minimum energy path calculations. *Physical Review B*, **2016**, 94,	3.3	63
165	Qualitative insight and quantitative analysis of the effect of temperature on the coercivity of a magnetic system. *AIP Advances*, **2016**, 6, 025213	1.5	7
164	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

163	Minimum energy path calculations with Gaussian process regression. *Nanosystems: Physics, Chemistry, Mathematics*, **2016**, 925-935	1.8	17
162	Tip-surface interaction and rate of magnetic transitions. *Journal of Physics: Conference Series*, **2016**, 741, 012184	0.3	
161	Crossover temperature for quantum tunnelling in spin systems. *Journal of Physics: Conference Series*, **2016**, 741, 012183	0.3	
160	Rate of thermal transitions in kagome spin ice. *Journal of Physics: Conference Series*, **2016**, 741, 012182	0.3	
159	Minimum energy path for the nucleation of misfit dislocations in Ge/Si(0 0 1) heteroepitaxy. *Modelling and Simulation in Materials Science and Engineering*, **2016**, 24, 035007	2	5
158	Classical to quantum mechanical tunneling mechanism crossover in thermal transitions between magnetic states. *Faraday Discussions*, **2016**, 195, 93-109	3.6	10
157	Charge localization in a diamine cation provides a test of energy functionals and self-interaction correction. *Nature Communications*, **2016**, 7, 11013	17.4	27
156	Efficient dynamical correction of the transition state theory rate estimate for a flat energy barrier. *Journal of Chemical Physics*, **2016**, 145, 094901	3.9	5
155	Application to large systems: general discussion. *Faraday Discussions*, **2016**,	3.6	4
154	Fundamentals: general discussion. *Faraday Discussions*, **2016**, 195, 139-169	3.6	2
153	Complex Orbitals, Multiple Local Minima, and Symmetry Breaking in Perdew-Zunger Self-Interaction Corrected Density Functional Theory Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 3195-207	6.4	39
152	Self-Interaction Corrected Functional Calculations of a Dipole-Bound Molecular Anion. *Journal of Physical Chemistry Letters*, **2016**, 7, 2068-73	6.4	9
151	Global transition path search for dislocation formation in Ge on Si(001). *Computer Physics Communications*, **2016**, 205, 13-21	4.2	203
150	Ultrafast structural pathway of charge transfer in n,n,n',n'-tetramethylethylenediamine. *Journal of Physical Chemistry A*, **2015**, 119, 2813-8	2.8	13
149	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
148	Long-Time-Scale Simulations of H2O Admolecule Diffusion on Ice Ih(0001) Surfaces. *Journal of Physical Chemistry C*, **2015**, 119, 16528-16536	3.8	13
147	Towards an Optimal Gradient-dependent Energy Functional of the PZ-SIC Form. *Procedia Computer Science*, **2015**, 51, 1858-1864	1.6	9
146	Improved Tight-Binding Charge Transfer Model and Calculations of Energetics of a Step on the Rutile TiO2(110) Surface. *Journal of Physical Chemistry C*, **2015**, 119, 10391-10399	3.8	3

145	Transition state theory approach to polymer escape from a one dimensional potential well. *Journal of Chemical Physics*, **2015**, 142, 224906	3.9	6
144	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
143	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
142	Computational Study of Electrochemical CO 2 Reduction at Transition Metal Electrodes. *Procedia Computer Science*, **2015**, 51, 1865-1871	1.6	23
141	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
140	Pipek-Mezey Orbital Localization Using Various Partial Charge Estimates. *Journal of Chemical Theory and Computation*, **2014**, 10, 642-9	6.4	49
139	Geothermal model calibration using a global minimization algorithm based on finding saddle points and minima of the objective function. *Computers and Geosciences*, **2014**, 65, 110-117	4.5	19
138	Catalytic Activity of Pt Nano-Particles for H2 Formation. *Topics in Catalysis*, **2014**, 57, 273-281	2.3	18
137	Improved initial guess for minimum energy path calculations. *Journal of Chemical Physics*, **2014**, 140, 214106	3.9	184
136	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
135	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
134	Calculations of magnetic states and minimum energy paths of transitions using a noncollinear extension of the Alexander-Anderson model and a magnetic force theorem. *Physical Review B*, **2014** , 89,	3.3	14
133	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
132	Polymer escape from a confining potential. *Journal of Chemical Physics*, **2014**, 140, 054907	3.9	2
131	EON: software for long time simulations of atomic scale systems. *Modelling and Simulation in Materials Science and Engineering*, **2014**, 22, 055002	2	49
130	Molecular reordering processes on ice (0001) surfaces from long timescale simulations. *Journal of Chemical Physics*, **2014**, 141, 234706	3.9	17
129	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
128	Adsorption of water dimer on platinum(111): identification of the -OH□□Pt hydrogen bond. *ACS Nano*, **2014**, 8, 11583-90	16.7	28

127	Effect of hydrogen adsorption on the magnetic properties of a surface nanocluster of iron. *Physical Review B*, **2013**, 88,	3.3	11
126	Unitary Optimization of Localized Molecular Orbitals. *Journal of Chemical Theory and Computation*, **2013**, 9, 5365-72	6.4	56
125	A transferable H2O interaction potential based on a single center multipole expansion: SCME. *Physical Chemistry Chemical Physics*, **2013**, 15, 16542-56	3.6	29
124	Hydrogen adsorption and desorption at the Pt(110)-(1□2) surface: experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2013**, 15, 6323-32	3.6	59
123	Size and shape dependence of thermal spin transitions in nanoislands. *Physical Review Letters*, **2013** , 110, 020604	7.4	26
122	Molecular rearrangement reactions in the gas phase triggered by electron attachment. *Physical Chemistry Chemical Physics*, **2013**, 15, 4754-66	3.6	19
121	Dynamics of basaltic glass dissolution □Capturing microscopic effects in continuum scale models. *Geochimica Et Cosmochimica Acta*, **2013**, 121, 311-327	5.5	24
120	Potential Energy Surfaces and Rates of Spin Transitions. *Zeitschrift Fur Physikalische Chemie*, **2013**, 1307080003[illegible]0008	[illegible]	[illegible]
119	Self-interaction corrected density functional calculations of molecular Rydberg states. *Journal of Chemical Physics*, **2013**, 139, 194102	3.9	29
118	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
117	Long-timescale simulations of diffusion in molecular solids. *Physical Chemistry Chemical Physics*, **2012**, 14, 10844-52	3.6	21
116	Adsorption of water monomer and clusters on platinum(111) terrace and related steps and kinks II. Surface diffusion. *Surface Science*, **2012**, 606, 233-238	1.8	14
115	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
114	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
113	A theoretical evaluation of possible transition metal electro-catalysts for N2 reduction. *Physical Chemistry Chemical Physics*, **2012**, 14, 1235-45	3.6	810
112	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
111	Simulated Annealing with Coarse Graining and Distributed Computing. *Lecture Notes in Computer Science*, **2012**, 34-44	0.9	17
110	Harmonic transition-state theory of thermal spin transitions. *Physical Review B*, **2012**, 85,	3.3	46

109	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 49-70	3.6	171
108	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
107	Reentrant mechanism for associative desorption: H2/Pt(110)-(1□2). *Physical Review Letters*, **2012**, 108, 156101	7.4	22
106	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
105	Optimization of Functionals of Orthonormal Functions in the Absence of Unitary Invariance. *Lecture Notes in Computer Science*, **2012**, 23-33	0.9	9
104	Path Optimization with Application to Tunneling. *Lecture Notes in Computer Science*, **2012**, 45-55	0.9	18
103	Efficient Sampling of Saddle Points with the Minimum-Mode Following Method. *SIAM Journal of Scientific Computing*, **2011**, 33, 633-652	2.6	22
102	Simulation of surface processes. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 944-9	11.5	90
101	Parallel implementation of Γ-point pseudopotential plane-wave DFT with exact exchange. *Journal of Computational Chemistry*, **2011**, 32, 54-69	3.5	42
100	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
99	Importance of complex orbitals in calculating the self-interaction-corrected ground state of atoms. *Physical Review A*, **2011**, 84,	2.6	67
98	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
97	Distributed implementation of the adaptive kinetic Monte Carlo method. *Mathematics and Computers in Simulation*, **2010**, 80, 1487-1498	3.3	17
96	Adsorption of water monomer and clusters on platinum(111) terrace and related steps and kinks. *Surface Science*, **2010**, 604, 1978-1986	1.8	52
95	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
94	Long time scale simulation of a grain boundary in copper. *New Journal of Physics*, **2009**, 11, 073034	2.9	20
93	Simulations of hydrogen diffusion at grain boundaries in aluminum. *Acta Materialia*, **2009**, 57, 4036-4045	8.4	69
92	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

91	Theoretical study of kinks on screw dislocation in silicon. *Physical Review B*, **2008**, 77,	3.3	41
90	Simulations of the fragmentation of the [V-H]⁻ anions as formed upon DEA to L-valine. *Journal of Physics: Conference Series*, **2008**, 115, 012014	0.3	2
89	Calculations of dislocation mobility using Nudged Elastic Band method and first principles DFT calculations. *Philosophical Magazine*, **2008**, 88, 91-100	1.6	23
88	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
87	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
86	Combined Experimental and Theoretical Study on the Nature and the Metastable Decay Pathways of the Amino Acid Ion Fragment [M−H]⁻. *Angewandte Chemie*, **2007**, 119, 8203-8205	3.6	1
85	Kinetic Monte Carlo simulations of Pd deposition and island growth on MgO(100). *Surface Science*, **2007**, 601, 3133-3142	1.8	35
84	Pd diffusion on MgO(100): The role of defects and small cluster mobility. *Surface Science*, **2006**, 600, 1351-1362	1.8	66
83	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
82	Predicting catalysis: understanding ammonia synthesis from first-principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 17719-35	3.4	168
81	A fast and robust algorithm for Bader decomposition of charge density. *Computational Materials Science*, **2006**, 36, 354-360	3.2	5896
80	Characterization of exciton self-trapping in amorphous silica. *Journal of Non-Crystalline Solids*, **2006**, 352, 2589-2595	3.9	22
79	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
78	Silica glass structure generation for ab initio calculations using small samples of amorphous silica. *Physical Review B*, **2005**, 71,	3.3	118
77	Cleavage and recovery of molecular water in silica. *Journal of Physical Chemistry B*, **2005**, 109, 10936-45	3.4	17
76	Optimization of hyperplanar transition states: Application to 2D test problems. *Computer Physics Communications*, **2005**, 169, 284-288	4.2	9
75	What determines the sticking probability of water molecules on ice?. *Physical Review Letters*, **2005**, 95, 223201	7.4	44
74	Comparison of methods for finding saddle points without knowledge of the final states. *Journal of Chemical Physics*, **2004**, 121, 9776-92	3.9	388

73	Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. *Journal of Physical Chemistry B*, **2004**, 108, 17886-17892	3.4	5882
72	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
71	An ab initio study of self-trapped excitons in □quartz. *Journal of Chemical Physics*, **2003**, 118, 6582-6593	3.9	31
70	Multiple time scale simulations of metal crystal growth reveal the importance of multiatom surface processes. *Physical Review Letters*, **2003**, 90, 116101	7.4	78
69	Theoretical Studies of Self-Diffusion and Dopant Clustering in Semiconductors. *Physica Status Solidi (B): Basic Research*, **2002**, 233, 24-30	1.3	18
68	Methods for Finding Saddle Points and Minimum Energy Paths **2002**, 269-302		84
67	Long-Time-Scale Simulations of Al(100) Crystal Growth **2002**, 63-74		
66	Theoretical calculations of dissociative adsorption of CH4 on an Ir(111) surface. *Physical Review Letters*, **2001**, 86, 664-7	7.4	124
65	Migration of O vacancies in □quartz: The effect of excitons and electron holes. *Physical Review B*, **2001**, 64,	3.3	35
64	Optimization of hyperplanar transition states. *Journal of Chemical Physics*, **2001**, 115, 9644-9656	3.9	42
63	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
62	Diffusion and Island formation on the ice Ih basal plane surface. *Computational Materials Science*, **2001**, 20, 325-336	3.2	50
61	Simulations of long time scale dynamics using the dimer method. *Materials Research Society Symposia Proceedings*, **2001**, 677, 811		4
60	Self-trapped excitons in quartz. *Nuclear Instruments & Methods in Physics Research B*, **2000**, 166-167, 451-458	1.2	17
59	Electric fields in ice and near water clusters. *Journal of Chemical Physics*, **2000**, 112, 3285-3292	3.9	51
58	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
57	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
56	Diffusion of Ge below the Si(100) surface: theory and experiment. *Physical Review Letters*, **2000**, 84, 2441-4	7.4	70

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