Hannes JÃ³nsson

List of Publications by Year
in descending order

Version: 2024-02-01

240 papers	59,819 citations	19608 61 h-index	1131 230 g-index
247 all docs	247 docs citations	247 times ranked	37223 citing authors

#	Article	IF	Citations
1	Lifetime of skyrmions in discrete systems with infinitesimal lattice constant. Journal of Magnetism and Magnetic Materials, 2022, 549, 168974.	1.0	5
2	Mechanism of Interlayer Transport on a Growing Au(111) Surface: 2D vs. 3D Growth. Surfaces and Interfaces, 2022, 31, 101944.	1.5	1
3	Simulations of the Electrochemical Oxidation of Pt Nanoparticles of Various Shapes. Journal of Physical Chemistry C, 2022, 126, 6773-6781.	1.5	5
4	Variational Density Functional Calculations of Excited States: Conical Intersection and Avoided Crossing in Ethylene Bond Twisting. Journal of Physical Chemistry Letters, 2022, 13, 3990-3999.	2.1	9
5	Indirect mechanism of Au adatom diffusion on the Si(100) surface. Physical Review B, 2022, 105, .	1.1	4
6	Reassignment of magic numbers for icosahedral Au clusters: 310, 564, 928 and 1426. Nanoscale, 2022, 14, 9053-9060.	2.8	3
7	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.	3.0	13
8	Localized and Delocalized States of a Diamine Cation: Resolution of a Controversy. Journal of Physical Chemistry Letters, 2021, 12, 1250-1255.	2.1	3
9	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.	2.1	7
10	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.	1.5	7
11	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.	2.3	12
12	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.	2.3	116
13	Elastic Collision Based Dynamic Partitioning Scheme for Hybrid Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5863-5875.	2.3	4
14	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.	2.3	9
15	Direct energy minimization based on exponential transformation in density functional calculations of finite and extended systems. Computer Physics Communications, 2021, 267, 108047.	3.0	7
16	Observation of Electric-Field-Induced Liberation of Guest Molecules from Clathrate Hydrate. Journal of Physical Chemistry Letters, 2021, 12, 10410-10416.	2.1	4
17	Simulations of the Oxidation and Degradation of Platinum Electrocatalysts. Small, 2020, 16, 1905159.	5.2	25
18	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.	1.3	25

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19	Minimum Mode Saddle Point Searches Using Gaussian Process Regression with Inverse-Distance Covariance Function. Journal of Chemical Theory and Computation, 2020, 16, 499-509.	2.3	15
20	Variational Density Functional Calculations of Excited States via Direct Optimization. Journal of Chemical Theory and Computation, 2020, 16, 6968-6982.	2.3	45
21	Stability of long-lived antiskyrmions in the Mn-Pt-Sn tetragonal Heusler material. Physical Review B, 2020, 102, .	1.1	9
22	Efficient optimization method for finding minimum energy paths of magnetic transitions. Journal of Physics Condensed Matter, 2020, 32, 345901.	0.7	12
23	Coupled quasimonopoles in chiral magnets. Physical Review B, 2020, 101, .	1.1	27
24	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
25	Variational calculations of excited states via direct optimization of the orbitals in DFT. Faraday Discussions, 2020, 224, 448-466.	1.6	31
26	Skyrmions in antiferromagnets: Thermal stability and the effect of external field and impurities. Journal of Applied Physics, 2020, 127, 213906.	1.1	19
27	Magnetic skyrmion annihilation by quantum mechanical tunneling. New Journal of Physics, 2020, 22, 083013.	1.2	6
28	Cuboctahedral Platinum Nanoparticles: Simulations of the Oxidation and Degradation of Platinum Electrocatalysts (Small 5/2020). Small, 2020, 16, 2070027.	5.2	1
29	Atomic and electronic structures of a vacancy in amorphous silicon. Physical Review B, 2020, 101, .	1.1	6
30	Exploring Potential Energy Surfaces with Saddle Point Searches. , 2020, , 689-714.		6
31	Fully self-consistent calculations of magnetic structure within non-collinear Alexander-Anderson model. Nanosystems: Physics, Chemistry, Mathematics, 2020, 11, 65-77.	0.2	2
32	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.	1.3	10
33	Nudged Elastic Band Calculations Accelerated with Gaussian Process Regression Based on Inverse Interatomic Distances. Journal of Chemical Theory and Computation, 2019, 15, 6738-6751.	2.3	44
34	Polarizable Embedding with a Transferable H₂O Potential Function I: Formulation and Tests on Dimer. Journal of Chemical Theory and Computation, 2019, 15, 6562-6577.	2.3	10
35	Polarizable Embedding with a Transferable H₂O Potential Function II: Application to (H₂O)_n Clusters and Liquid Water. Journal of Chemical Theory and Computation, 2019, 15, 6578-6587.	2.3	9
36	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.	1.5	71

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37	Density functional theory calculations and thermodynamic analysis of bridgmanite surface structure. Physical Chemistry Chemical Physics, 2019, 21, 1009-1013.	1.3	3
38	Spirit : Multifunctional framework for atomistic spin simulations. Physical Review B, 2019, 99, .	1.1	112
39	R-NEB: Accelerated Nudged Elastic Band Calculations by Use of Reflection Symmetry. Journal of Chemical Theory and Computation, 2019, 15, 3215-3222.	2.3	23
40	Effect of H adsorption on the magnetic properties of an Fe island on a W(110) surface. Physical Review B, 2019, 100, .	1.1	1
41	Determination of the structure and properties of an edge dislocation in rutile TiO2. Acta Materialia, 2019, 163, 199-207.	3.8	27
42	Density Functional Theory Calculations and Thermodynamic Analysis of the Forsterite Mg₂SiO₄(010) Surface. Journal of Physical Chemistry C, 2019, 123, 464-472.	1.5	13
43	Reassignment of â€˜magic numbersâ€™ for Au clusters of decahedral and FCC structural motifs. Nanoscale, 2018, 10, 5124-5132.	2.8	23
44	Lifetime of racetrack skyrmions. Scientific Reports, 2018, 8, 3433.	1.6	127
45	Calculations of Product Selectivity in Electrochemical CO₂ Reduction. ACS Catalysis, 2018, 8, 5240-5249.	5.5	203
46	Efficient evaluation of atom tunneling combined with electronic structure calculations. Journal of Chemical Physics, 2018, 148, 102334.	1.2	23
47	Energy surface and lifetime of magnetic skyrmions. Journal of Magnetism and Magnetic Materials, 2018, 459, 236-240.	1.0	33
48	The effect of confinement and defects on the thermal stability of skyrmions. Physica B: Condensed Matter, 2018, 549, 6-9.	1.3	31
49	Duplication, Collapse, and Escape of Magnetic Skyrmions Revealed Using a Systematic Saddle Point Search Method. Physical Review Letters, 2018, 121, 197202.	2.9	36
50	Reply to: â€œThe diamine cation is not a chemical example where density functional theory failsâ€• Nature Communications, 2018, 9, 5348.	5.8	5
51	Exploring Potential Energy Surfaces with Saddle Point Searches. , 2018, , 1-26.		2
52	Models of the energy landscape for an element of shakti spin ice. Nanosystems: Physics, Chemistry, Mathematics, 2018, 9, 711-715.	0.2	0
53	Atomic scale simulations of heterogeneous electrocatalysis: recent advances. Advances in Physics: X, 2017, 2, 481-495.	1.5	18
54	Optimal atomic structure of amorphous silicon obtained from density functional theory calculations. New Journal of Physics, 2017, 19, 063018.	1.2	32

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55	Theory and Applications of Generalized Pipekâ€“Mezey Wannier Functions. Journal of Chemical Theory and Computation, 2017, 13, 460-474.	2.3	32
56	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.	1.5	17
57	Improved Minimum Mode Following Method for Finding First Order Saddle Points. Journal of Chemical Theory and Computation, 2017, 13, 125-134.	2.3	23
58	Nudged elastic band calculations accelerated with Gaussian process regression. Journal of Chemical Physics, 2017, 147, 152720.	1.2	109
59	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.	2.3	32
60	Ultrafast X-ray absorption study of longitudinalâ€“transverse phonon coupling in electrolyte aqueous solution. Physical Chemistry Chemical Physics, 2017, 19, 27266-27274.	1.3	2
61	Coherence in nonradiative transitions: internal conversion in Rydberg-excited N-methyl and N-ethyl morpholine. Physical Chemistry Chemical Physics, 2017, 19, 26403-26411.	1.3	22
62	Atomic Scale Formation Mechanism of Edge Dislocation Relieving Lattice Strain in a GeSi overlayer on Si(001). Scientific Reports, 2017, 7, 11966.	1.6	13
63	Observation of Structural Wavepacket Motion: The Umbrella Mode in Rydberg-Excited N-Methyl Morpholine. Journal of Physical Chemistry Letters, 2017, 8, 3740-3744.	2.1	20
64	Magnetic exchange force microscopy: theoretical analysis of induced magnetization reversals. Nanoscale, 2017, 9, 13320-13325.	2.8	12
65	First-principles Green's-function method for surface calculations: A pseudopotential localized basis set approach. Physical Review B, 2017, 96, .	1.1	211
66	Energy surface and transition rates in a hexagonal element of spin ice. Journal of Physics: Conference Series, 2017, 903, 012006.	0.3	0
67	The effect of temperature and external field on transitions in elements of kagome spin ice. New Journal of Physics, 2017, 19, 113008.	1.2	9
68	Calculations of the onset temperature for tunneling in multispin systems. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 454-461.	0.2	4
69	Truncated minimum energy path method for finding first order saddle points. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 586-595.	0.2	9
70	Instantons describing tunneling between magnetic states at finite temperature. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 746-759.	0.2	2
71	Thermal stability of magnetic states in submicron magnetic islands. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 572-578.	0.2	1
72	Calculations of switching field and energy barrier for magnetic islands with perpendicular anisotropy. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 701-708.	0.2	0

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73	Nanocluster structure deduced from AC-STEM images coupled to theoretical modelling. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 723-731.	0.2	0
74	Tip-surface interaction and rate of magnetic transitions. Journal of Physics: Conference Series, 2016, 741, 012184.	0.3	0
75	Crossover temperature for quantum tunnelling in spin systems. Journal of Physics: Conference Series, 2016, 741, 012183.	0.3	1
76	Rate of thermal transitions in kagome spin ice. Journal of Physics: Conference Series, 2016, 741, 012182.	0.3	0
77	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.	0.8	7
78	Classical to quantum mechanical tunneling mechanism crossover in thermal transitions between magnetic states. Faraday Discussions, 2016, 195, 93-109.	1.6	13
79	Charge localization in a diamine cation provides a test of energy functionals and self-interaction correction. Nature Communications, 2016, 7, 11013.	5.8	37
80	Efficient dynamical correction of the transition state theory rate estimate for a flat energy barrier. Journal of Chemical Physics, 2016, 145, 094901.	1.2	5
81	Application to large systems: general discussion. Faraday Discussions, 2016, 195, 671-698.	1.6	4
82	Fundamentals: general discussion. Faraday Discussions, 2016, 195, 139-169.	1.6	2
83	Complex Orbitals, Multiple Local Minima, and Symmetry Breaking in Perdewâ€“Zunger Self-Interaction Corrected Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2016, 12, 3195-3207.	2.3	54
84	Self-Interaction Corrected Functional Calculations of a Dipole-Bound Molecular Anion. Journal of Physical Chemistry Letters, 2016, 7, 2068-2073.	2.1	14
85	Global transition path search for dislocation formation in Ge on Si(001). Computer Physics Communications, 2016, 205, 13-21.	3.0	299
86	Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdewâ€“Zunger Self-Interaction Correction to Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 4296-4302.	2.3	29
87	Mechanism and activation energy of magnetic skyrmion annihilation obtained from minimum energy path calculations. Physical Review B, 2016, 94, .	1.1	83
88	Qualitative insight and quantitative analysis of the effect of temperature on the coercivity of a magnetic system. AIP Advances, 2016, 6, 025213.	0.6	10
89	Faraday efficiency and mechanism of electrochemical surface reactions: CO₂ reduction and H₂ formation on Pt(111). Faraday Discussions, 2016, 195, 619-636.	1.6	45
90	Minimum energy path calculations with Gaussian process regression. Nanosystems: Physics, Chemistry, Mathematics, 2016, , 925-935.	0.2	23

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91	Computational Study of Electrochemical CO2 Reduction at Transition Metal Electrodes. Procedia Computer Science, 2015, 51, 1865-1871.	1.2	26
92	Removing External Degrees of Freedom from Transition-State Search Methods using Quaternions. Journal of Chemical Theory and Computation, 2015, 11, 1055-1062.	2.3	21
93	Ultrafast Structural Pathway of Charge Transfer in N,N,Nâ€²,Nâ€²-Tetramethylethylenediamine. Journal of Physical Chemistry A, 2015, 119, 2813-2818.	1.1	15
94	Method for finding mechanism and activation energy of magnetic transitions, applied to skyrmion and antivortex annihilation. Computer Physics Communications, 2015, 196, 335-347.	3.0	160
95	Long-Time-Scale Simulations of H₂O Admolecule Diffusion on Ice Ih(0001) Surfaces. Journal of Physical Chemistry C, 2015, 119, 16528-16536.	1.5	15
96	Towards an Optimal Gradient-dependent Energy Functional of the PZ-SIC Form. Procedia Computer Science, 2015, 51, 1858-1864.	1.2	12
97	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.	1.5	8
98	Transition state theory approach to polymer escape from a one dimensional potential well. Journal of Chemical Physics, 2015, 142, 224906.	1.2	7
99	Calculations of Al dopant inÎ±-quartz using a variational implementation of the Perdewâ€“Zunger self-interaction correction. New Journal of Physics, 2015, 17, 083006.	1.2	26
100	Magic-Number Gold Nanoclusters with Diameters from 1 to 3.5 nm: Relative Stability and Catalytic Activity for CO Oxidation. Nano Letters, 2015, 15, 682-688.	4.5	92
101	EON: software for long time simulations of atomic scale systems. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 055002.	0.8	58
102	Molecular reordering processes on ice (0001) surfaces from long timescale simulations. Journal of Chemical Physics, 2014, 141, 234706.	1.2	17
103	Self-interaction corrected density functional calculations of Rydberg states of molecular clusters: N,N-dimethylisopropylamine. Journal of Chemical Physics, 2014, 141, 234308.	1.2	22
104	Adsorption of Water Dimer on Platinum(111): Identification of the â^'OHÂ·Â·Â·Pt Hydrogen Bond. ACS Nano, 2014, 8, 11583-11590.	7.3	34
105	Pipekâ€“Mezey Orbital Localization Using Various Partial Charge Estimates. Journal of Chemical Theory and Computation, 2014, 10, 642-649.	2.3	73
106	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.	2.0	22
107	Catalytic Activity of Pt Nano-Particles for H2 Formation. Topics in Catalysis, 2014, 57, 273-281.	1.3	26
108	Improved initial guess for minimum energy path calculations. Journal of Chemical Physics, 2014, 140, 214106.	1.2	279

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109	Ultrafast structural dynamics in Rydberg excited N,N,Nâ€²,Nâ€²-tetramethylethylenediamine: conformation dependent electron lone pair interaction and charge delocalization. Chemical Science, 2014, 5, 4394-4403.	3.7	31
110	Variational, Self-Consistent Implementation of the Perdewâ€“Zunger Self-Interaction Correction with Complex Optimal Orbitals. Journal of Chemical Theory and Computation, 2014, 10, 5324-5337.	2.3	69
111	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, .	1.1	17
112	Effect of Magnetic States on the Reactivity of an FCC(111) Iron Surface. Journal of Physical Chemistry C, 2014, 118, 15863-15873.	1.5	14
113	Polymer escape from a confining potential. Journal of Chemical Physics, 2014, 140, 054907.	1.2	2
114	Effect of hydrogen adsorption on the magnetic properties of a surface nanocluster of iron. Physical Review B, 2013, 88, .	1.1	12
115	Unitary Optimization of Localized Molecular Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 5365-5372.	2.3	69
116	A transferable H2O interaction potential based on a single center multipole expansion: SCME. Physical Chemistry Chemical Physics, 2013, 15, 16542.	1.3	32
117	Hydrogen adsorption and desorption at the Pt(110)-(1Ã—2) surface: experimental and theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 6323.	1.3	67
118	Size and Shape Dependence of Thermal Spin Transitions in Nanoislands. Physical Review Letters, 2013, 110, 020604.	2.9	32
119	Molecular rearrangement reactions in the gas phase triggered by electron attachment. Physical Chemistry Chemical Physics, 2013, 15, 4754.	1.3	25
120	Dynamics of basaltic glass dissolution â€“ Capturing microscopic effects in continuum scale models. Geochimica Et Cosmochimica Acta, 2013, 121, 311-327.	1.6	29
121	Self-interaction corrected density functional calculations of molecular Rydberg states. Journal of Chemical Physics, 2013, 139, 194102.	1.2	32
122	Local density of states analysis using Bader decomposition for N2 and CO2 adsorbed on Pt(110)-(1â€‰Ã—â€‰2) electrodes. Journal of Chemical Physics, 2012, 137, 164705.	1.2	39
123	Reentrant Mechanism for Associative Desorption<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:mi>Pt</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo stretchy="false">)</mml:mo><mml:mtext mathvariant="normal">â^’</mml:mtext><mml:mo		

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127	Adsorption of water monomer and clusters on platinum(111) terrace and related steps and kinks II. Surface diffusion. Surface Science, 2012, 606, 233-238.	0.8	15
128	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.	1.2	25
129	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.	1.4	40
130	A theoretical evaluation of possible transition metal electro-catalysts for N₂reduction. Physical Chemistry Chemical Physics, 2012, 14, 1235-1245.	1.3	1,184
131	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.	2.3	131
132	Simulated Annealing with Coarse Graining and Distributed Computing. Lecture Notes in Computer Science, 2012, , 34-44.	1.0	17
133	Harmonic transition-state theory of thermal spin transitions. Physical Review B, 2012, 85, .	1.1	77
134	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. Physical Chemistry Chemical Physics, 2012, 14, 49-70.	1.3	198
135	Optimization of Functionals of Orthonormal Functions in the Absence of Unitary Invariance. Lecture Notes in Computer Science, 2012, , 23-33.	1.0	9
136	Path Optimization with Application to Tunneling. Lecture Notes in Computer Science, 2012, , 45-55.	1.0	22
137	Experimental and theoretical study of the metastable decay of negatively charged nucleosides in the gas phase. Physical Chemistry Chemical Physics, 2011, 13, 15283.	1.3	19
138	Efficient Sampling of Saddle Points with the Minimum-Mode Following Method. SIAM Journal of Scientific Computing, 2011, 33, 633-652.	1.3	23
139	Simulation of surface processes. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 944-949.	3.3	93
140	Parallel implementation of Î³â€point pseudopotential planeâ€wave DFT with exact exchange. Journal of Computational Chemistry, 2011, 32, 54-69.	1.5	47
141	Importance of complex orbitals in calculating the self-interaction-corrected ground state of atoms. Physical Review A, 2011, 84, .	1.0	75
142	Distributed implementation of the adaptive kinetic Monte Carlo method. Mathematics and Computers in Simulation, 2010, 80, 1487-1498.	2.4	17
143	Adsorption of water monomer and clusters on platinum(111) terrace and related steps and kinks. Surface Science, 2010, 604, 1978-1986.	0.8	61
144	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.	1.5	990

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145	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.	0.7	15
146	Long time scale simulation of a grain boundary in copper. New Journal of Physics, 2009, 11, 073034.	1.2	20
147	Simulations of hydrogen diffusion at grain boundaries in aluminum. Acta Materialia, 2009, 57, 4036-4045.	3.8	78
148	Comparison of Quantum Dynamics and Quantum Transition State Theory Estimates of the H + CH₄ Reaction Rate. Journal of Physical Chemistry A, 2009, 113, 4468-4478.	1.1	140
149	The Effect of Co-adsorbed Water on the Stability and Configuration of Formyl (HCO) and Hydroxymethylidyne (COH) Intermediates on Pt(111): A Density Functional Theory Study. ECS Transactions, 2009, 16, 621-626.	0.3	1
150	Calculations of dislocation mobility using Nudged Elastic Band method and first principles DFT calculations. Philosophical Magazine, 2008, 88, 91-100.	0.7	24
151	Theoretical study of kinks on screw dislocation in silicon. Physical Review B, 2008, 77, .	1.1	49
152	Simulations of the fragmentation of the [V-H]^{â^'}anions as formed upon DEA to L-valine. Journal of Physics: Conference Series, 2008, 115, 012014.	0.3	2
153	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, 3241-3250.	1.3	678
154	Combined Experimental and Theoretical Study on the Nature and the Metastable Decay Pathways of the Amino Acid Ion Fragment [Mâ^'H]^{â^'}. Angewandte Chemie - International Edition, 2007, 46, 8057-8059.	7.2	47
155	Kinetic Monte Carlo simulations of Pd deposition and island growth on MgO(100). Surface Science, 2007, 601, 3133-3142.	0.8	37
156	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192
157	A fast and robust algorithm for Bader decomposition of charge density. Computational Materials Science, 2006, 36, 354-360.	1.4	7,727
158	Characterization of exciton self-trapping in amorphous silica. Journal of Non-Crystalline Solids, 2006, 352, 2589-2595.	1.5	29
159	Pd diffusion on MgO(100): The role of defects and small cluster mobility. Surface Science, 2006, 600, 1351-1362.	0.8	66
160	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.	1.2	156
161	Optimization of hyperplanar transition states: Application to 2D test problems. Computer Physics Communications, 2005, 169, 284-288.	3.0	9
162	What Determines the Sticking Probability of Water Molecules on Ice?. Physical Review Letters, 2005, 95, 223201.	2.9	48

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163	Small Pd Clusters, up to the Tetramer At Least, Are Highly Mobile on the MgO(100) Surface. Physical Review Letters, 2005, 95, 146103.	2.9	87
164	Silica glass structure generation forab initiocalculations using small samples of amorphous silica. Physical Review B, 2005, 71, .	1.1	134
165	Cleavage and Recovery of Molecular Water in Silica. Journal of Physical Chemistry B, 2005, 109, 10936-10945.	1.2	18
166	Comparison of methods for finding saddle points without knowledge of the final states. Journal of Chemical Physics, 2004, 121, 9776-9792.	1.2	462
167	Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. Journal of Physical Chemistry B, 2004, 108, 17886-17892.	1.2	8,672
168	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.	0.6	24
169	An ab initio study of self-trapped excitons in Î±-quartz. Journal of Chemical Physics, 2003, 118, 6582-6593.	1.2	34
170	Multiple Time Scale Simulations of Metal Crystal Growth Reveal the Importance of Multiatom Surface Processes. Physical Review Letters, 2003, 90, 116101.	2.9	86
171	Methods for Finding Saddle Points and Minimum Energy Paths. , 2002, , 269-302.		133
172	Theoretical Studies of Self-Diffusion and Dopant Clustering in Semiconductors. Physica Status Solidi (B): Basic Research, 2002, 233, 24-30.	0.7	21
173	Long-Time-Scale Simulations of Al(100) Crystal Growth. , 2002, , 63-74.		0
174	Long time scale kinetic Monte Carlo simulations without lattice approximation and predefined event table. Journal of Chemical Physics, 2001, 115, 9657-9666.	1.2	398
175	Diffusion and Island formation on the ice Ih basal plane surface. Computational Materials Science, 2001, 20, 325-336.	1.4	54
176	Simulations of long time scale dynamics using the dimer method. Materials Research Society Symposia Proceedings, 2001, 677, 811.	0.1	4
177	Theoretical Calculations of Dissociative Adsorption ofCH4on an Ir(111) Surface. Physical Review Letters, 2001, 86, 664-667.	2.9	136
178	Migration of O vacancies in Î±-quartz: The effect of excitons and electron holes. Physical Review B, 2001, 64, .	1.1	39
179	Optimization of hyperplanar transition states. Journal of Chemical Physics, 2001, 115, 9644-9656.	1.2	43
180	Self-trapped excitons in quartz. Nuclear Instruments & Methods in Physics Research B, 2000, 166-167, 451-458.	0.6	20

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