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	A climbing image nudged elastic band method for finding saddle points and minimum energy paths. Journal of Chemical Physics, 2000, 113, 9901-9904.	1.2	15,067
2	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
3	A fast and robust algorithm for Bader decomposition of charge density. Computational Materials Science, 2006, 36, 354-360.	1.4	7,727
4	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.	1.2	7,115
5	A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives. Journal of Chemical Physics, 1999, 111, 7010-7022.	1.2	2,505
6	Reversible work transition state theory: application to dissociative adsorption of hydrogen. Surface Science, 1995, 324, 305-337.	0.8	1,953
7	A theoretical evaluation of possible transition metal electro-catalysts for N₂reduction. Physical Chemistry Chemical Physics, 2012, 14, 1235-1245.	1.3	1,184
8	Nudged elastic band method for finding minimum energy paths of transitions. , 1998, , .		1,161
9	Systematic analysis of local atomic structure combined with 3D computer graphics. Computational Materials Science, 1994, 2, 279-286.	1.4	1,077
10	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
11	Quantum and thermal effects inH2dissociative adsorption: Evaluation of free energy barriers in multidimensional quantum systems. Physical Review Letters, 1994, 72, 1124-1127.	2.9	762
12	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
13	Icosahedral Ordering in the Lennard-Jones Liquid and Glass. Physical Review Letters, 1988, 60, 2295-2298.	2.9	497
14	Comparison of methods for finding saddle points without knowledge of the final states. Journal of Chemical Physics, 2004, 121, 9776-9792.	1.2	462
15	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
16	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
17	Structural changes accompanying densification of random hard-sphere packings. Physical Review E, 1993, 47, 3975-3984.	0.8	360
18	Global transition path search for dislocation formation in Ge on Si(001). Computer Physics Communications, 2016, 205, 13-21.	3.0	299

#	Article	IF	Citations
19	Improved initial guess for minimum energy path calculations. Journal of Chemical Physics, 2014, 140, 214106.	1.2	279
20	First-principles Green's-function method for surface calculations: A pseudopotential localized basis set approach. Physical Review B, 2017, 96, .	1.1	211
21	Calculations of Product Selectivity in Electrochemical CO₂ Reduction. ACS Catalysis, 2018, 8, 5240-5249.	5.5	203
22	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. Physical Chemistry Chemical Physics, 2012, 14, 49-70.	1.3	198
23	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192
24	Molecular multipole moments of water molecules in ice Ih. Journal of Chemical Physics, 1998, 109, 4546-4551.	1.2	167
25	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
26	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
27	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
28	Theoretical Calculations of Dissociative Adsorption ofCH4on an Ir(111) Surface. Physical Review Letters, 2001, 86, 664-667.	2.9	136
29	Silica glass structure generation forab initiocalculations using small samples of amorphous silica. Physical Review B, 2005, 71, .	1.1	134
30	Methods for Finding Saddle Points and Minimum Energy Paths. , 2002, , 269-302.		133
31	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
32	Diffusion mechanisms relevant to metal crystal growth: Pt/Pt(111). Surface Science, 1994, 317, 15-36.	0.8	127
33	Lifetime of racetrack skyrmions. Scientific Reports, 2018, 8, 3433.	1.6	127
34	THEORETICALSTUDIES OFATOMIC-SCALEPROCESSESRELEVANT TOCRYSTALGROWTH. Annual Review of Physical Chemistry, 2000, 51, 623-653.	4.8	121
35	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
36	Investigation of the reliability of density functional methods: Reaction and activation energies for Siâ€“Si bond cleavage and H2 elimination from silanes. Journal of Chemical Physics, 1996, 104, 148-158.	1.2	112

#	Article	IF	Citations
37	Spirit : Multifunctional framework for atomistic spin simulations. Physical Review B, 2019, 99, .	1.1	112
38	Nudged elastic band calculations accelerated with Gaussian process regression. Journal of Chemical Physics, 2017, 147, 152720.	1.2	109
39	Generalized path integral based quantum transition state theory. Chemical Physics Letters, 1997, 278, 91-96.	1.2	105
40	Experimental and Theoretical Study of the Rotation of Si Ad-dimers on the Si(100) Surface. Physical Review Letters, 1996, 77, 2518-2521.	2.9	102
41	Atomistic Determination of Cross-Slip Pathway and Energetics. Physical Review Letters, 1997, 79, 3676-3679.	2.9	98
42	Multipole moments of water molecules in clusters and ice Ih from first principles calculations. Journal of Chemical Physics, 1999, 111, 6011-6015.	1.2	98
43	Simulation of surface processes. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 944-949.	3.3	93
44	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
45	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.	1.2	89
46	Thermal Diffusion Processes in Metal-Tip-Surface Interactions: Contact Formation and Adatom Mobility. Physical Review Letters, 1996, 77, 5067-5070.	2.9	87
47	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
48	Multiple Time Scale Simulations of Metal Crystal Growth Reveal the Importance of Multiatom Surface Processes. Physical Review Letters, 2003, 90, 116101.	2.9	86
49	Mechanism and activation energy of magnetic skyrmion annihilation obtained from minimum energy path calculations. Physical Review B, 2016, 94, .	1.1	83
50	Diffusion of Ge below the Si(100) Surface: Theory and Experiment. Physical Review Letters, 2000, 84, 2441-2444.	2.9	78
51	Simulations of hydrogen diffusion at grain boundaries in aluminum. Acta Materialia, 2009, 57, 4036-4045.	3.8	78
52	Harmonic transition-state theory of thermal spin transitions. Physical Review B, 2012, 85, .	1.1	77
53	Importance of complex orbitals in calculating the self-interaction-corrected ground state of atoms. Physical Review A, 2011, 84, .	1.0	75
54	Pipekâ€“Mezey Orbital Localization Using Various Partial Charge Estimates. Journal of Chemical Theory and Computation, 2014, 10, 642-649.	2.3	73

#	Article	IF	Citations
55	Reversible work based quantum transition state theory. Journal of Chemical Physics, 1994, 101, 8964-8971.	1.2	72
56	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.	1.2	71
57	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
58	Unitary Optimization of Localized Molecular Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 5365-5372.	2.3	69
59	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
60	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
61	Excess energy of grain-boundary trijunctions: an atomistic simulation study. Acta Materialia, 1999, 47, 2821-2829.	3.8	66
62	Pd diffusion on MgO(100): The role of defects and small cluster mobility. Surface Science, 2006, 600, 1351-1362.	0.8	66
63	Atomic structure of Î²-SiC(100) surfaces: an ab initio study. Surface Science, 1995, 330, 265-275.	0.8	65
64	Adsorption of water monomer and clusters on platinum(111) terrace and related steps and kinks. Surface Science, 2010, 604, 1978-1986.	0.8	61
65	EON: software for long time simulations of atomic scale systems. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 055002.	0.8	58
66	Diffusion and Island formation on the ice Ih basal plane surface. Computational Materials Science, 2001, 20, 325-336.	1.4	54
67	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
68	Structure and molecular properties of adsorbates at low coverage: Light-atom scattering from adsorbed Xe and CO. Physical Review B, 1984, 30, 2241-2244.	1.1	52
69	Twoâ€•and threeâ€•body forces in the interaction of He atoms with Xe overlayers adsorbed on (0001) graphite. Journal of Chemical Physics, 1989, 91, 6477-6493.	1.2	52
70	Electric fields in ice and near water clusters. Journal of Chemical Physics, 2000, 112, 3285-3292.	1.2	52
71	Low-temperature homoepitaxial growth of Pt(111) in simulated vapor deposition. Physical Review B, 1994, 49, 2208-2211.	1.1	49
72	Theoretical study of kinks on screw dislocation in silicon. Physical Review B, 2008, 77, .	1.1	49

#	Article	IF	Citations
73	What Determines the Sticking Probability of Water Molecules on Ice?. Physical Review Letters, 2005, 95, 223201.	2.9	48
74	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
75	Parallel implementation of Î³â€point pseudopotential planeâ€wave DFT with exact exchange. Journal of Computational Chemistry, 2011, 32, 54-69.	1.5	47
76	Dimer and String Formation during Low Temperature Silicon Deposition on Si(100). Physical Review Letters, 1996, 77, 1326-1329.	2.9	45
77	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
78	Variational Density Functional Calculations of Excited States via Direct Optimization. Journal of Chemical Theory and Computation, 2020, 16, 6968-6982.	2.3	45
79	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
80	Light atom scattering from adsorbates at low coverage. Surface Science, 1984, 148, 126-138.	0.8	43
81	Optimization of hyperplanar transition states. Journal of Chemical Physics, 2001, 115, 9644-9656.	1.2	43
82	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
83	Migration of O vacancies in Î±-quartz: The effect of excitons and electron holes. Physical Review B, 2001, 64, .	1.1	39
84	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
85	Kinetic Monte Carlo simulations of Pd deposition and island growth on MgO(100). Surface Science, 2007, 601, 3133-3142.	0.8	37
86	Charge localization in a diamine cation provides a test of energy functionals and self-interaction correction. Nature Communications, 2016, 7, 11013.	5.8	37
87	A Computational Exercise Illustrating Molecular Vibrations and Normal Modes. The Chemical Educator, 1998, 3, 1-17.	0.0	36
88	Duplication, Collapse, and Escape of Magnetic Skyrmions Revealed Using a Systematic Saddle Point Search Method. Physical Review Letters, 2018, 121, 197202.	2.9	36
89	Atomic structure of Î²-SiC(100) surfaces: a study using the Tersoff potential. Surface Science, 1994, 316, 181-188.	0.8	34
90	An ab initio study of self-trapped excitons in Î±-quartz. Journal of Chemical Physics, 2003, 118, 6582-6593.	1.2	34

#	Article	IF	Citations
91	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
92	Hydrogen atom scattering from physisorbed overlayers. Surface Science, 1985, 155, 499-534.	0.8	33
93	Energy surface and lifetime of magnetic skyrmions. Journal of Magnetism and Magnetic Materials, 2018, 459, 236-240.	1.0	33
94	A transferable H2O interaction potential based on a single center multipole expansion: SCME. Physical Chemistry Chemical Physics, 2013, 15, 16542.	1.3	32
95	Size and Shape Dependence of Thermal Spin Transitions in Nanoislands. Physical Review Letters, 2013, 110, 020604.	2.9	32
96	Self-interaction corrected density functional calculations of molecular Rydberg states. Journal of Chemical Physics, 2013, 139, 194102.	1.2	32
97	Optimal atomic structure of amorphous silicon obtained from density functional theory calculations. New Journal of Physics, 2017, 19, 063018.	1.2	32
98	Theory and Applications of Generalized Pipekâ€“Mezey Wannier Functions. Journal of Chemical Theory and Computation, 2017, 13, 460-474.	2.3	32
99	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
100	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
101	The effect of confinement and defects on the thermal stability of skyrmions. Physica B: Condensed Matter, 2018, 549, 6-9.	1.3	31
102	Variational calculations of excited states via direct optimization of the orbitals in DFT. Faraday Discussions, 2020, 224, 448-466.	1.6	31
103	Absorption and Resonance Raman Study of the2B1(X)â˜2A2(A) Transition of Chlorine Dioxide in the Gas Phase. Journal of Physical Chemistry A, 1999, 103, 1748-1757.	1.1	30
104	Atomic exchange processes in sputter deposition of Pt on Pt(111). Surface Science, 1995, 324, 35-46.	0.8	29
105	Characterization of exciton self-trapping in amorphous silica. Journal of Non-Crystalline Solids, 2006, 352, 2589-2595.	1.5	29
106	Dynamics of basaltic glass dissolution â€“ Capturing microscopic effects in continuum scale models. Geochimica Et Cosmochimica Acta, 2013, 121, 311-327.	1.6	29
107	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
108	Determination of the structure and properties of an edge dislocation in rutile TiO2. Acta Materialia, 2019, 163, 199-207.	3.8	27

#	Article	IF	Citations
109	Coupled quasimonopoles in chiral magnets. Physical Review B, 2020, 101, .	1.1	27
110	Catalytic Activity of Pt Nano-Particles for H2 Formation. Topics in Catalysis, 2014, 57, 273-281.	1.3	26
111	Computational Study of Electrochemical CO2 Reduction at Transition Metal Electrodes. Procedia Computer Science, 2015, 51, 1865-1871.	1.2	26
112	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
113	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
114	Molecular rearrangement reactions in the gas phase triggered by electron attachment. Physical Chemistry Chemical Physics, 2013, 15, 4754.	1.3	25
115	Simulations of the Oxidation and Degradation of Platinum Electrocatalysts. Small, 2020, 16, 1905159.	5.2	25
116	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
117	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
118	Calculations of dislocation mobility using Nudged Elastic Band method and first principles DFT calculations. Philosophical Magazine, 2008, 88, 91-100.	0.7	24
119	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		

#	Article	IF	Citations
127	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
128	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
129	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
130	Path Optimization with Application to Tunneling. Lecture Notes in Computer Science, 2012, , 45-55.	1.0	22
131	On the laterally averaged interaction potential between He atoms and the (0001) surface of graphite. Chemical Physics Letters, 1986, 129, 139-143.	1.2	21
132	A parallel implementation of the Car-Parrinello method by orbital decomposition. Computer Physics Communications, 1994, 81, 1-18.	3.0	21
133	Parallel short-range molecular dynamics using the Ä€dhÄ•a runtime system. Computer Physics Communications, 1997, 102, 28-43.	3.0	21
134	Theoretical Studies of Self-Diffusion and Dopant Clustering in Semiconductors. Physica Status Solidi (B): Basic Research, 2002, 233, 24-30.	0.7	21
135	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
136	Atom scattering as a quantitative surface probe: Noble-gas monolayer and bilayer adsorbed on graphite. Physical Review B, 1984, 30, 4203-4206.	1.1	20
137	Molecular dynamics simulations of a pressureâ€induced glass transition. Journal of Chemical Physics, 1995, 102, 1796-1805.	1.2	20
138	Elastic sheet method for identifying atoms in molecules. Journal of Chemical Physics, 1999, 111, 10664-10669.	1.2	20
139	Self-trapped excitons in quartz. Nuclear Instruments & Methods in Physics Research B, 2000, 166-167, 451-458.	0.6	20
140	Long time scale simulation of a grain boundary in copper. New Journal of Physics, 2009, 11, 073034.	1.2	20
141	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
142	A hybrid decomposition parallel implementation of the Car-Parrinello method. Computer Physics Communications, 1995, 87, 319-340.	3.0	19
143	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
144	Skyrmions in antiferromagnets: Thermal stability and the effect of external field and impurities. Journal of Applied Physics, 2020, 127, 213906.	1.1	19

#	Article	IF	Citations
145	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.	0.6	18
146	Cleavage and Recovery of Molecular Water in Silica. Journal of Physical Chemistry B, 2005, 109, 10936-10945.	1.2	18
147	Atomic scale simulations of heterogeneous electrocatalysis: recent advances. Advances in Physics: X, 2017, 2, 481-495.	1.5	18
148	Distributed implementation of the adaptive kinetic Monte Carlo method. Mathematics and Computers in Simulation, 2010, 80, 1487-1498.	2.4	17
149	Simulated Annealing with Coarse Graining and Distributed Computing. Lecture Notes in Computer Science, 2012, , 34-44.	1.0	17
150	Molecular reordering processes on ice (0001) surfaces from long timescale simulations. Journal of Chemical Physics, 2014, 141, 234706.	1.2	17
151	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
152	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
153	Elastic scattering of light atoms from physisorbed overlayers. What are the non-additive many-body corrections?. Faraday Discussions of the Chemical Society, 1985, 80, 29-45.	2.2	16
154	Many-Body Corrections to the Intermolecular Interaction Probed with Atom-Surface Scattering. Physical Review Letters, 1986, 57, 412-415.	2.9	15
155	Low energy He atom scattering from Ag(110) and Ag(111): Is there an effective two-body potential?. Surface Science, 1987, 181, 495-508.	0.8	15
156	Dynamic-domain-decomposition parallel molecular dynamics. Computer Physics Communications, 1997, 102, 44-58.	3.0	15
157	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
158	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
159	Potential Energy Surfaces and Rates of Spin Transitions. Zeitschrift Fur Physikalische Chemie, 0, , 130708000310008.	1.4	15
160	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
161	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
162	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

#	Article	IF	Citations
163	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
164	Self-Interaction Corrected Functional Calculations of a Dipole-Bound Molecular Anion. Journal of Physical Chemistry Letters, 2016, 7, 2068-2073.	2.1	14
165	He atom scattering from the graphite (0001) surface: Diffraction peaks, resonance splittings, and isolated resonances. Journal of Chemical Physics, 1987, 86, 3711-3719.	1.2	13
166	RAW quantum transition state theory. , 1998, , .		13
167	Classical to quantum mechanical tunneling mechanism crossover in thermal transitions between magnetic states. Faraday Discussions, 2016, 195, 93-109.	1.6	13
168	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
169	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
170	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
171	Effect of hydrogen adsorption on the magnetic properties of a surface nanocluster of iron. Physical Review B, 2013, 88, .	1.1	12
172	Towards an Optimal Gradient-dependent Energy Functional of the PZ-SIC Form. Procedia Computer Science, 2015, 51, 1858-1864.	1.2	12
173	Magnetic exchange force microscopy: theoretical analysis of induced magnetization reversals. Nanoscale, 2017, 9, 13320-13325.	2.8	12
174	Efficient optimization method for finding minimum energy paths of magnetic transitions. Journal of Physics Condensed Matter, 2020, 32, 345901.	0.7	12
175	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
176	Hydrogen atom scattering from physisorbed overlayers. Surface Science, 1987, 180, 353-370.	0.8	11
177	Self-trapped excitons at the quartz(0001) surface. Faraday Discussions, 2000, 117, 303-311.	1.6	11
178	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
179	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
180	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

#	Article	IF	Citations
181	Optimization of hyperplanar transition states: Application to 2D test problems. Computer Physics Communications, 2005, 169, 284-288.	3.0	9
182	A method for finding the ridge between saddle points applied to rare event rate estimates. Physical Chemistry Chemical Physics, 2012, 14, 2884.	1.3	9
183	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
184	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
185	Stability of long-lived antiskyrmions in the Mn-Pt-Sn tetragonal Heusler material. Physical Review B, 2020, 102, .	1.1	9
186	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
187	Optimization of Functionals of Orthonormal Functions in the Absence of Unitary Invariance. Lecture Notes in Computer Science, 2012, , 23-33.	1.0	9
188	Truncated minimum energy path method for finding first order saddle points. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 586-595.	0.2	9
189	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
190	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
191	Transition state theory approach to polymer escape from a one dimensional potential well. Journal of Chemical Physics, 2015, 142, 224906.	1.2	7
192	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
193	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
194	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
195	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
196	Structural variations in strained crystalline multilayers. Journal of Materials Research, 1994, 9, 2190-2197.	1.2	6
197	Magnetic skyrmion annihilation by quantum mechanical tunneling. New Journal of Physics, 2020, 22, 083013.	1.2	6
198	Atomic and electronic structures of a vacancy in amorphous silicon. Physical Review B, 2020, 101, .	1.1	6

#	Article	IF	Citations
199	Exploring Potential Energy Surfaces with Saddle Point Searches. , 2020, , 689-714.		6
200	Summary Abstract: Comparison of theory and experiment for scattering of He from CO adsorbed on Au(111) at low coverage. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1985, 3, 1665-1667.	0.9	5
201	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
202	Reply to: â€œThe diamine cation is not a chemical example where density functional theory failsâ€• Nature Communications, 2018, 9, 5348.	5.8	5
203	Lifetime of skyrmions in discrete systems with infinitesimal lattice constant. Journal of Magnetism and Magnetic Materials, 2022, 549, 168974.	1.0	5
204	Simulations of the Electrochemical Oxidation of Pt Nanoparticles of Various Shapes. Journal of Physical Chemistry C, 2022, 126, 6773-6781.	1.5	5
205	Simulations of long time scale dynamics using the dimer method. Materials Research Society Symposia Proceedings, 2001, 677, 811.	0.1	4
206	Application to large systems: general discussion. Faraday Discussions, 2016, 195, 671-698.	1.6	4
207	Elastic Collision Based Dynamic Partitioning Scheme for Hybrid Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5863-5875.	2.3	4
208	Calculations of the onset temperature for tunneling in multispin systems. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 454-461.	0.2	4
209	Observation of Electric-Field-Induced Liberation of Guest Molecules from Clathrate Hydrate. Journal of Physical Chemistry Letters, 2021, 12, 10410-10416.	2.1	4
210	Indirect mechanism of Au adatom diffusion on the Si(100) surface. Physical Review B, 2022, 105, .	1.1	4
211	Research-Level Computers and Software in the Undergraduate Curriculum. Journal of Chemical Education, 1995, 72, 332.	1.1	3
212	Exploring the Excited States of Vacancy Defects in Silica. Materials Research Society Symposia Proceedings, 1998, 540, 379.	0.1	3
213	Density functional theory calculations and thermodynamic analysis of bridgmanite surface structure. Physical Chemistry Chemical Physics, 2019, 21, 1009-1013.	1.3	3
214	Localized and Delocalized States of a Diamine Cation: Resolution of a Controversy. Journal of Physical Chemistry Letters, 2021, 12, 1250-1255.	2.1	3
215	Reassignment of magic numbers for icosahedral Au clusters: 310, 564, 928 and 1426. Nanoscale, 2022, 14, 9053-9060.	2.8	3
216	Summary Abstract: Helium scattering from W(001). Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1987, 5, 790-791.	0.9	2

#	Article	IF	Citations
217	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
218	Polymer escape from a confining potential. Journal of Chemical Physics, 2014, 140, 054907.	1.2	2
219	Fundamentals: general discussion. Faraday Discussions, 2016, 195, 139-169.	1.6	2
220	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
221	Exploring Potential Energy Surfaces with Saddle Point Searches. , 2018, , 1-26.		2
222	Instantons describing tunneling between magnetic states at finite temperature. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 746-759.	0.2	2
223	Fully self-consistent calculations of magnetic structure within non-collinear Alexander-Anderson model. Nanosystems: Physics, Chemistry, Mathematics, 2020, 11, 65-77.	0.2	2
224	Silicon AD-Dimer Binding on Si(100). Materials Research Society Symposia Proceedings, 1995, 389, 35.	0.1	1
225	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
226	Crossover temperature for quantum tunnelling in spin systems. Journal of Physics: Conference Series, 2016, 741, 012183.	0.3	1
227	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
228	Cuboctahedral Platinum Nanoparticles: Simulations of the Oxidation and Degradation of Platinum Electrocatalysts (Small 5/2020). Small, 2020, 16, 2070027.	5.2	1
229	Thermal stability of magnetic states in submicron magnetic islands. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 572-578.	0.2	1
230	Mechanism of Interlayer Transport on a Growing Au(111) Surface: 2D vs. 3D Growth. Surfaces and Interfaces, 2022, 31, 101944.	1.5	1
231	Structure and Properties of Strained Crystalline Multilayers. Materials Research Society Symposia Proceedings, 1994, 351, 349.	0.1	0
232	Vacancy Migration Barrier Energetics and Pathways in Silica. Materials Research Society Symposia Proceedings, 1998, 538, 317.	0.1	0
233	Tip-surface interaction and rate of magnetic transitions. Journal of Physics: Conference Series, 2016, 741, 012184.	0.3	0
234	Rate of thermal transitions in kagome spin ice. Journal of Physics: Conference Series, 2016, 741, 012182.	0.3	0

#	Article	IF	Citations
235	Energy surface and transition rates in a hexagonal element of spin ice. Journal of Physics: Conference Series, 2017, 903, 012006.	0.3	0
236	COMPUTATIONAL STUDIES OF SELF-TRAPPED EXCITONS IN SILICA. , 2000, , 329-337.		0
237	Long-Time-Scale Simulations of Al(100) Crystal Growth. , 2002, , 63-74.		0
238	Calculations of switching field and energy barrier for magnetic islands with perpendicular anisotropy. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 701-708.	0.2	0
239	Nanocluster structure deduced from AC-STEM images coupled to theoretical modelling. Nanosystems: Physics, Chemistry, Mathematics, 2017, , 723-731.	0.2	0
240	Models of the energy landscape for an element of shakti spin ice. Nanosystems: Physics, Chemistry, Mathematics, 2018, 9, 711-715.	0.2	0