

G-J Kroes

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papers

6,149
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45
h-index

70
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157
ext. papers

6,481
ext. citations

5
avg, IF

6.18
L-index

#	Paper	IF	Citations
150	Chemically accurate simulation of a prototypical surface reaction: H ₂ dissociation on Cu(111). <i>Science</i> , 2009 , 326, 832-4	33.3	282
149	Atomic and molecular hydrogen interacting with Pt(111). <i>Journal of Chemical Physics</i> , 1999 , 111, 11155-11163	31.63	176
148	Reactive and nonreactive scattering of H ₂ from a metal surface is electronically adiabatic. <i>Science</i> , 2006 , 312, 86-9	33.3	173
147	Predicting catalysis: understanding ammonia synthesis from first-principles calculations. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 17719-35	3.4	168
146	Quantum theory of dissociative chemisorption on metal surfaces. <i>Accounts of Chemical Research</i> , 2002 , 35, 193-200	24.3	154
145	Constructing accurate potential energy surfaces for a diatomic molecule interacting with a solid surface: H ₂ +Pt(111) and H ₂ +Cu(100). <i>Journal of Chemical Physics</i> , 2002 , 116, 3841-3855	3.9	127
144	Quantum and classical dynamics of reactive scattering of H ₂ from metal surfaces. <i>Chemical Society Reviews</i> , 2016 , 45, 3658-700	58.5	116
143	Ab Initio Molecular Dynamics Calculations versus Quantum-State-Resolved Experiments on CHD ₃ + Pt(111): New Insights into a Prototypical Gas-Surface Reaction. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 1294-9	6.4	112
142	Six-Dimensional Quantum Dynamics of Dissociative Chemisorption of (v=0, j=0) H ₂ on Cu(100). <i>Physical Review Letters</i> , 1997 , 78, 3583-3586	7.4	109
141	Reactive and diffractive scattering of H ₂ from Pt(111) studied using a six-dimensional wave packet method. <i>Journal of Chemical Physics</i> , 2002 , 117, 5885-5898	3.9	107
140	Theoretical Study of Stable, Defect-Free (TiO ₂) _n Nanoparticles with n = 10-16. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 16808-16817	3.8	106
139	An analytical six-dimensional potential energy surface for dissociation of molecular hydrogen on Cu(100). <i>Journal of Chemical Physics</i> , 1996 , 104, 7344-7358	3.9	106
138	Accurate Neural Network Description of Surface Phonons in Reactive Gas-Surface Dynamics: N + Ru(0001). <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2131-2136	6.4	103
137	Frontiers in surface scattering simulations. <i>Science</i> , 2008 , 321, 794-7	33.3	101
136	Electronic friction dominates hydrogen hot-atom relaxation on Pd(100). <i>Physical Review Letters</i> , 2014 , 112, 103203	7.4	97
135	Chemically Accurate Simulation of a Polyatomic Molecule-Metal Surface Reaction. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2402-6	6.4	93
134	Effect of surface motion on the rotational quadrupole alignment parameter of D ₂ reacting on Cu(111). <i>Physical Review Letters</i> , 2012 , 108, 236104	7.4	89

133	Multidimensional effects on dissociation of N ₂ on Ru(0001). <i>Physical Review Letters</i> , 2006 , 96, 096102	7.4	85
132	Six-dimensional dynamics study of reactive and non reactive scattering of H ₂ from Cu(111) using a chemically accurate potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 6499-519	3.6	82
131	Application of the modified Shepard interpolation method to the determination of the potential energy surface for a molecule-surface reaction: H ₂ + Pt(111). <i>Journal of Chemical Physics</i> , 2004 , 120, 2392-404	3.9	81
130	Theoretical calculation of the energy of formation of LiBH ₄ . <i>Chemical Physics Letters</i> , 2005 , 405, 73-78	2.5	79
129	SIX-DIMENSIONAL DYNAMICS OF DISSOCIATIVE CHEMISORPTION OF H ₂ ON METAL SURFACES. <i>Journal of Theoretical and Computational Chemistry</i> , 2005 , 04, 493-581	1.8	76
128	Dissociative chemisorption of methane on metal surfaces: tests of dynamical assumptions using quantum models and ab initio molecular dynamics. <i>Journal of Chemical Physics</i> , 2014 , 141, 054102	3.9	75
127	Towards chemically accurate simulation of molecule-surface reactions. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 14966-81	3.6	73
126	Six-dimensional quantum dynamics of dissociative chemisorption of H ₂ on Cu(100). <i>Journal of Chemical Physics</i> , 1997 , 107, 3309-3323	3.9	68
125	In-plane and out-of-plane diffraction of H ₂ from metal surfaces. <i>Physical Review Letters</i> , 2004 , 93, 246104	4.4	68
124	SBH10: A Benchmark Database of Barrier Heights on Transition Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 19807-19815	3.8	67
123	Reactive scattering of H ₂ from Cu(100): comparison of dynamics calculations based on the specific reaction parameter approach to density functional theory with experiment. <i>Journal of Chemical Physics</i> , 2013 , 138, 044708	3.9	66
122	Surface Reaction Barriometry: Methane Dissociation on Flat and Stepped Transition-Metal Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 4177-4182	6.4	64
121	Quantum dynamics of dissociative chemisorption of CH ₄ on Ni(111): Influence of the bending vibration. <i>Journal of Chemical Physics</i> , 2010 , 133, 144308	3.9	64
120	Six-dimensional quantum dynamics of scattering of (v=0, j=0) H ₂ from Pt(111): comparison to experiment and to classical dynamics results. <i>Chemical Physics Letters</i> , 2001 , 347, 277-284	2.5	63
119	Dissociation of H ₂ on Cu(100): Dynamics on a new two-dimensional potential energy surface. <i>Journal of Chemical Physics</i> , 1995 , 102, 3873-3883	3.9	63
118	Toward a Database of Chemically Accurate Barrier Heights for Reactions of Molecules with Metal Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4106-14	6.4	61
117	Six-dimensional quantum dynamics of dissociative chemisorption of H ₂ on Ru(0001). <i>Journal of Chemical Physics</i> , 2005 , 122, 44701	3.9	59
116	Molecular dynamics simulations of the ice temperature dependence of water ice photodesorption. <i>Journal of Chemical Physics</i> , 2010 , 132, 184510	3.9	56

115	Rovibrationally inelastic scattering of ($v=1, j=1$) H ₂ from Cu(100): Experiment and theory. <i>Journal of Chemical Physics</i> , 2001 , 114, 495	3.9	56
114	Multi-dimensional potential energy surface determination by modified Shepard interpolation for a molecule-surface reaction: H ₂ + Pt(1 1 1). <i>Chemical Physics Letters</i> , 2003 , 376, 566-575	2.5	54
113	The effect of the exchange-correlation functional on H ₂ dissociation on Ru(0001). <i>Journal of Chemical Physics</i> , 2014 , 140, 084702	3.9	51
112	Hydrogen dissociation on Cu(111): the influence of lattice motion. Part I. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 4552-61	3.6	50
111	Competition between vibrational excitation and dissociation in collisions of H ₂ with Cu(100). <i>Physical Review B</i> , 1996 , 53, 10397-10401	3.3	49
110	New results for the OH ($\nu = 0, j = 0$) + CO ($\nu = 0, j = 0$) \rightarrow H + CO ₂ reaction: Five- and full-dimensional quantum dynamical study on several potential energy surfaces. <i>Journal of Chemical Physics</i> , 2004 , 120, 4263-72	3.9	48
109	Rotational effects in dissociation of H ₂ on Pd(111): Quantum and classical study. <i>Journal of Chemical Physics</i> , 2003 , 119, 12553-12562	3.9	48
108	Dynamics on Six-Dimensional Potential Energy Surfaces for H ₂ /Cu(111): Corrugation Reducing Procedure versus Modified Shepard Interpolation Method and PW91 versus RPBE. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 11192-11201	3.8	47
107	Six-dimensional quantum dynamics of scattering of ($v=0, j=0$) H ₂ and D ₂ from Cu(111): test of two LEPS potential energy surfaces. <i>Chemical Physics Letters</i> , 2002 , 360, 390-399	2.5	47
106	Application of an efficient asymptotic analysis method to molecule-surface scattering. <i>Journal of Chemical Physics</i> , 1995 , 103, 1216-1225	3.9	47
105	Apparent failure of the Born-Oppenheimer static surface model for vibrational excitation of molecular hydrogen on copper. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 20881-6	11.5	45
104	Methane dissociation on Pt(111): Searching for a specific reaction parameter density functional. <i>Journal of Chemical Physics</i> , 2016 , 144, 044702	3.9	45
103	Quasiharmonic approximation applied to LiBH ₄ and its decomposition products. <i>Physical Review B</i> , 2006 , 73,	3.3	44
102	Thermal lattice expansion effect on reactive scattering of H ₂ from Cu(111) at T(s) = 925 K. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 8770-81	2.8	43
101	Accurate Probabilities for Highly Activated Reaction of Polyatomic Molecules on Surfaces Using a High-Dimensional Neural Network Potential: CHD + Cu(111). <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 1763-1768	6.4	42
100	Adiabatic Energy Loss in Hyperthermal H Atom Collisions with Cu and Au: A Basis for Testing the Importance of Nonadiabatic Energy Loss. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3735-3740	6.4	42
99	Enigmatic HCl + Au(111) Reaction: A Puzzle for Theory and Experiment. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 25760-25779	3.8	40
98	Vibrational deexcitation and rotational excitation of H ₂ and D ₂ scattered from Cu(111): adiabatic versus non-adiabatic dynamics. <i>Journal of Chemical Physics</i> , 2012 , 137, 064707	3.9	40

97	Reactive and nonreactive scattering of N ₂ from Ru(0001): a six-dimensional adiabatic study. <i>Journal of Chemical Physics</i> , 2006 , 125, 114706	3.9	40
96	Performance of a Non-Local van der Waals Density Functional on the Dissociation of H ₂ on Metal Surfaces. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 12146-58	2.8	37
95	Diffusion Monte Carlo for Accurate Dissociation Energies of 3d Transition Metal Containing Molecules. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2583-97	6.4	37
94	Ab initio molecular dynamics calculations on scattering of hyperthermal H atoms from Cu(111) and Au(111). <i>Journal of Chemical Physics</i> , 2014 , 141, 054705	3.9	37
93	Dissociative chemisorption of methane on Ni(111) using a chemically accurate fifteen dimensional potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 30540-30550	3.6	36
92	The influence of surface motion on the direct subsurface absorption of H ₂ on Pd(111). <i>Journal of Chemical Physics</i> , 1997 , 107, 10652-10661	3.9	36
91	Dissociative chemisorption of H ₂ on the Cu(110) surface: a quantum and quasiclassical dynamical study. <i>Journal of Chemical Physics</i> , 2007 , 127, 164722	3.9	36
90	Chemically accurate simulation of dissociative chemisorption of D ₂ on Pt(1 1 1). <i>Chemical Physics Letters</i> , 2017 , 683, 329-335	2.5	33
89	Orbital-Dependent Electronic Friction Significantly Affects the Description of Reactive Scattering of N from Ru(0001). <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2957-2962	6.4	33
88	Signatures of site-specific reaction of H ₂ on Cu(100). <i>Journal of Chemical Physics</i> , 2002 , 117, 6673-6687	3.9	33
87	Quantum dynamics of the dissociation of H ₂ on Cu(100): dependence of the site-reactivity on initial rovibrational state. <i>Faraday Discussions</i> , 2000 , 109-32; discussion 161-89	3.6	33
86	Diffraction and reactive scattering of H ₂ from Ru(0001): experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 8583-97	3.6	32
85	Molecular knife throwing: aiming for dissociation at specific surface sites through state-selection. <i>Chemical Physics Letters</i> , 2000 , 328, 317-324	2.5	31
84	The effect of corrugation on the quantum dynamics of dissociative and diffractive scattering of H ₂ from Pt(111). <i>Journal of Chemical Physics</i> , 2000 , 113, 8300-8312	3.9	31
83	Dissociation and recombination of D ₂ on Cu(111): ab initio molecular dynamics calculations and improved analysis of desorption experiments. <i>Journal of Chemical Physics</i> , 2014 , 141, 124705	3.9	30
82	Accuracy of trajectory methods for activated adsorption of H ₂ on Cu(100). <i>Chemical Physics Letters</i> , 1998 , 296, 515-520	2.5	30
81	Diffractive and reactive scattering of (v=0, j=0) HD from Pt(111): Six-dimensional quantum dynamics compared with experiment. <i>Journal of Chemical Physics</i> , 2003 , 118, 4190-4197	3.9	30
80	Rotational Effects on Vibrational Excitation of H ₂ on Cu(100). <i>Physical Review Letters</i> , 1999 , 82, 1410-1414	3.4	30

79	Performance of a fully close-coupled wave packet method for the H ₂ +LiF(001) model problem. <i>Journal of Chemical Physics</i> , 1995 , 102, 5512-5524	3.9	30
78	Performance of close-coupled wave packet methods for molecule-corrugated surface scattering. <i>Journal of Chemical Physics</i> , 1995 , 103, 5121-5136	3.9	29
77	Dissociative and diffractive scattering of H ₂ from Pt(111): A four-dimensional quantum dynamics study. <i>Journal of Chemical Physics</i> , 2002 , 116, 9435-9448	3.9	28
76	A classical study of rotational effects in dissociation of H ₂ on Cu(100). <i>Physical Chemistry Chemical Physics</i> , 1999 , 1, 1359-1374	3.6	28
75	Surface Temperature Effects on Dissociative Chemisorption of H ₂ on Cu(100). <i>Journal of Physical Chemistry C</i> , 2013 , 117, 8851-8863	3.8	27
74	A classical dynamics method for H ₂ diffraction from metal surfaces. <i>Journal of Chemical Physics</i> , 2005 , 122, 154706	3.9	27
73	Theoretical Reaction Dynamics Study of the Effect of Vibrational Excitation of CO on the OH + CO → H + CO ₂ Reaction. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 8672-8681	2.8	27
72	Six-dimensional quantum dynamics of (v=0,j=0)D ₂ and of (v=1,j=0)H ₂ scattering from Cu(111). <i>Journal of Chemical Physics</i> , 2005 , 122, 214709	3.9	27
71	Theoretical rate constants for the OH+CO→H+CO ₂ reaction using variational transition state theory on analytical potential energy surfaces. <i>Journal of Chemical Physics</i> , 2002 , 117, 8736-8744	3.9	27
70	A general method for controlling and resolving rotational orientation of molecules in molecule-surface collisions. <i>Nature Communications</i> , 2017 , 8, 15357	17.4	26
69	Sticking of HCl to ice at hyperthermal energies: Dependence on incidence energy, incidence angle, and surface temperature. <i>Journal of Chemical Physics</i> , 2001 , 115, 482-491	3.9	26
68	Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 8962-9048	3.6	26
67	Full-dimensional quantum initial state-selected reaction probabilities (J=0) for the reaction OH(v=0,j=0)+CO(v=0,j=0)→CO ₂ +H. <i>Chemical Physics Letters</i> , 2002 , 352, 281-287	2.5	25
66	Quantum Monte Carlo Calculations on a Benchmark Molecule-Metal Surface Reaction: H + Cu(111). <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3208-3219	6.4	24
65	Quantum dynamical study of the H ₂ and D ₂ dissociative adsorption and diffraction from the NiAl(110) alloy surface. <i>Physical Review B</i> , 2006 , 73,	3.3	24
64	Anomalous Dependence of the Reactivity on the Presence of Steps: Dissociation of D on Cu(211). <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 170-175	6.4	23
63	Reactive scattering of H ₂ from Cu(100): six-dimensional quantum dynamics results for reaction and scattering obtained with a new, accurately fitted potential-energy surface. <i>Journal of Chemical Physics</i> , 2004 , 121, 11379-87	3.9	23
62	Vibrational Excitation of H Scattering from Cu(111): Effects of Surface Temperature and of Allowing Energy Exchange with the Surface. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 13617-13633	3.8	22

61	Rotational effects on the dissociation dynamics of CHD3 on Pt(111). <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 8174-85	3.6	22
60	Multiconfiguration time-dependent Hartree method applied to molecular dissociation on surfaces: H2 + Pt(111). <i>Journal of Chemical Physics</i> , 2006 , 124, 74706	3.9	22
59	Quantum and classical dynamics of H2 scattering from Pd(111) at off-normal incidence. <i>Physical Review B</i> , 2005 , 72,	3.3	22
58	The HD isotope effect in the stability of lithium alanate. <i>Chemical Physics Letters</i> , 2006 , 423, 102-105	2.5	21
57	Role of CO vibration in the complex-forming OH+CO->H+CO2 reaction. <i>Physical Review A</i> , 2004 , 70,	2.6	21
56	Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 2287-2299	3.8	21
55	Specific Reaction Parameter Density Functional Based on the Meta-Generalized Gradient Approximation: Application to H + Cu(111) and H + Ag(111). <i>Journal of Physical Chemistry A</i> , 2019 , 123, 5395-5406	2.8	20
54	Density Functional Theory for Molecule-Metal Surface Reactions: When Does the Generalized Gradient Approximation Get It Right, and What to Do If It Does Not. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 10552-10560	6.4	20
53	Theoretical Investigation of Two H2 Molecules Inside the Cages of the Structure H Clathrate Hydrate. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 21664-21672	3.8	20
52	Calculations on rotationally and diffractively inelastic molecule-surface scattering for arbitrary angles of incidence: A new wave packet technique. <i>Journal of Chemical Physics</i> , 1994 , 101, 805-813	3.9	19
51	Dynamics of H dissociation on the close-packed (111) surface of the noblest metal: H + Au(111). <i>Journal of Chemical Physics</i> , 2016 , 145, 144701	3.9	19
50	Effect of Transition Metal Dopants on Initial Mass Transport in the Dehydrogenation of NaAlH4: Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 3-14	3.8	18
49	Modeling surface motion effects in N2 dissociation on W(110): Ab initio molecular dynamics calculations and generalized Langevin oscillator model. <i>Journal of Chemical Physics</i> , 2016 , 144, 244708	3.9	18
48	N2 dissociation on W(110): An ab initio molecular dynamics study on the effect of phonons. <i>Journal of Chemical Physics</i> , 2015 , 142, 104702	3.9	17
47	Dynamics of dissociative adsorption of hydrogen on a CO-precovered Ru(0001) surface: a comparison of theoretical and experimental results. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 1331-40	3.6	17
46	A Theoretical Study of H2 Reacting on Ti/Al(100) Surfaces. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 11027-11034	3.8	17
45	Toward Detection of Electron-Hole Pair Excitation in H-atom Collisions with Au(111): Adiabatic Molecular Dynamics with a Semi-Empirical Full-Dimensional Potential Energy Surface. <i>Zeitschrift Fur Physikalische Chemie</i> , 2013 , 227,	3.1	16
44	Chebyshev high-dimensional model representation (Chebyshev-HDMR) potentials: application to reactive scattering of H2 from Pt(111) and Cu(111) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 8628-43	3.6	16

43	Converged five-dimensional quantum calculations for OH+CO->H+CO2. <i>Journal of Chemical Physics</i> , 2002 , 116, 4184-4191	3.9	16
42	Transferability of the Specific Reaction Parameter Density Functional for H + Pt(111) to H + Pt(211). <i>Journal of Physical Chemistry C</i> , 2019 , 123, 2973-2986	3.8	16
41	Incident Angle Dependence of CHD Dissociation on the Stepped Pt(211) Surface. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 19652-19660	3.8	15
40	Quantum Dynamics of Dissociative Chemisorption of H on the Stepped Cu(211) Surface. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 23049-23063	3.8	15
39	H2 Diffraction from a Strained Pseudomorphic Monolayer of Cu Deposited on Ru(0001). <i>Journal of Physical Chemistry C</i> , 2012 , 116, 13671-13678	3.8	15
38	Identifying spectator bonds in modeling reactions: OH+CO->H+CO2. <i>Chemical Physics Letters</i> , 2006 , 417, 43-47	2.5	15
37	Transferability of the SRP32-vdW specific reaction parameter functional to CHD dissociation on Pt(110)-(2 × 1). <i>Journal of Chemical Physics</i> , 2019 , 150, 124702	3.9	14
36	Towards a specific reaction parameter density functional for reactive scattering of H2 from Pd(111). <i>Journal of Chemical Physics</i> , 2013 , 139, 244707	3.9	14
35	Using n-mode potentials for reactive scattering: Application to the 6D H2 + Pt(1 1 1) problem. <i>Chemical Physics Letters</i> , 2007 , 440, 334-340	2.5	14
34	CHD dissociation on Pt(111): A comparison of the reaction dynamics based on the PBE functional and on a specific reaction parameter functional. <i>Journal of Chemical Physics</i> , 2018 , 149, 044701	3.9	14
33	7D Quantum Dynamics of H2 Scattering from Cu(111): The Accuracy of the Phonon Sudden Approximation. <i>Zeitschrift Fur Physikalische Chemie</i> , 2013 , 130617035227002	3.1	13
32	Six-dimensional quasiclassical and quantum dynamics of H2 dissociation on the c(2 × 2)-Ti/Al(100) surface. <i>Journal of Chemical Physics</i> , 2011 , 134, 114708	3.9	13
31	Closing the Gap Between Experiment and Theory: Reactive Scattering of HCl from Au(111). <i>Journal of Physical Chemistry C</i> , 2020 , 124, 15944-15960	3.8	12
30	Dynamics of H2 dissociation on the 1/2 ML c(2 × 2)-Ti/Al(100) surface. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 3234-47	3.6	12
29	Application of van der Waals functionals to the calculation of dissociative adsorption of N2 on W(110) for static and dynamic systems. <i>Journal of Chemical Physics</i> , 2016 , 144, 084702	3.9	12
28	Dissociation of CHD on Cu(111), Cu(211), and single atom alloys of Cu(111). <i>Journal of Chemical Physics</i> , 2018 , 149, 224701	3.9	12
27	Methane on a stepped surface: Dynamical insights on the dissociation of CHD on Pt(111) and Pt(211). <i>Journal of Chemical Physics</i> , 2018 , 149, 094701	3.9	12
26	HOD on Ni(111): molecular dynamics prediction of molecular beam experiments. <i>Journal of Chemical Physics</i> , 2018 , 149, 244706	3.9	11

25	Analysis of Energy Dissipation Channels in a Benchmark System of Activated Dissociation: N on Ru(0001). <i>Journal of Physical Chemistry C</i> , 2018 , 122, 23470-23480	3.8	11
24	CHD3 Dissociation on the Kinked Pt(210) Surface: A Comparison of Experiment and Theory. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 14530-14539	3.8	10
23	Assessment of Two Problems of Specific Reaction Parameter Density Functional Theory: Sticking and Diffraction of H on Pt(111). <i>Journal of Physical Chemistry C</i> , 2019 , 123, 10406-10418	3.8	9
22	Toward a Specific Reaction Parameter Density Functional for H ₂ + Ni(111): Comparison of Theory with Molecular Beam Sticking Experiments. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 20420-20433	3.8	9
21	Curious Mechanism of the Dissociative Chemisorption of Ammonia on Ru(0001). <i>Journal of Physical Chemistry C</i> , 2019 , 123, 28291-28300	3.8	9
20	Test of the Transferability of the Specific Reaction Parameter Functional for H + Cu(111) to D + Ag(111). <i>Journal of Physical Chemistry C</i> , 2018 , 122, 22939-22952	3.8	9
19	Dynamical Study of the Dissociative Chemisorption of CHD on Pd(111). <i>Journal of Physical Chemistry C</i> , 2019 , 123, 24013-24023	3.8	8
18	Quantum Monte Carlo calculations on dissociative chemisorption of H + Al(110): Minimum barrier heights and their comparison to DFT values. <i>Journal of Chemical Physics</i> , 2020 , 153, 224701	3.9	8
17	An AIMD study of dissociative chemisorption of methanol on Cu(111) with implications for formaldehyde formation. <i>Journal of Chemical Physics</i> , 2019 , 150, 024706	3.9	8
16	Density functional embedding for periodic and nonperiodic diffusion Monte Carlo calculations. <i>Physical Review B</i> , 2018 , 98,	3.3	7
15	Possible effect of static surface disorder on diffractive scattering of H from Ru(0001): Comparison between theory and experiment. <i>Journal of Chemical Physics</i> , 2017 , 147, 244705	3.9	7
14	Efficient penetration of the basal plane (0001) face of ice Ih by HF at T _s =150 K: dependence on incidence energy, incidence angle, and rotational energy. <i>Journal of Chemical Physics</i> , 2004 , 120, 11796-803	3.9	7
13	Performance and application of a symmetry adapted pseudo spectral method for scattering of a diatomic molecule from a square surface: H ₂ + Cu(1 0 0). <i>Chemical Physics</i> , 2004 , 304, 59-77	2.3	7
12	The dependence of dissociative chemisorption of H ₂ on Pd(1 1 1) on H ₂ rotation: a six-dimensional quantum dynamics study. <i>Chemical Physics Letters</i> , 2004 , 393, 166-172	2.5	6
11	Designing new SRP density functionals including non-local vdW-DF2 correlation for H + Cu(111) and their transferability to H + Ag(111), Au(111) and Pt(111). <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 7875-7901	3.6	6
10	Predictions on the effect of initial molecular orientation and rotation on penetration of the (0001) face of hexagonal ice by HCl. <i>Chemical Physics Letters</i> , 2003 , 376, 581-587	2.5	5
9	Exploring surface landscapes with molecules: rotationally induced diffraction of H on LiF(001) under fast grazing incidence conditions. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 16317-16322	3.6	4
8	A theoretical study of H(2) dissociation on (sq.rt(3) x sq.rt(3))R30 degrees CO/Ru(0001). <i>Journal of Chemical Physics</i> , 2010 , 132, 144704	3.9	4

7	H ₂ /LiF(001) diffractive scattering under fast grazing incidence using a DFT-based potential energy surface. <i>Physical Review B</i> , 2017 , 96,	3.3	3
6	Theory of Molecular Scattering from and Photochemistry at Ice Surfaces. <i>Proceedings of the International Astronomical Union</i> , 2005 , 1, 427	0.1	3
5	Performance of Made Simple Meta-GGA Functionals with rVV10 Nonlocal Correlation for H + Cu(111), D + Ag(111), H + Au(111), and D + Pt(111). <i>Journal of Physical Chemistry C</i> , 2021 , 125, 8993-9010 ^{3.8}		3
4	An ab initio molecular dynamics study of D ₂ dissociation on CO-precovered Ru(0001). <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 21190-201	3.6	3
3	Assessing density functionals for describing methane dissociative chemisorption on Pt(110)-(2x1) surface. <i>Chinese Journal of Chemical Physics</i> , 2021 , 34, 883-895	0.9	1
2	Highly Efficient Activation of HCl Dissociation on Au(111) via Rotational Preexcitation. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 7252-7260	6.4	0
1	Three-dimensional Langevin dynamics of N atom scattering from N-covered Ag(1 1 1). <i>Chemical Physics</i> , 2022 , 560, 111557	2.3	