# G-J Kroes

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 150 papers | 6,149 citations | 45 h-index | 70 g-index |
| 157 ext. papers | 6,481 ext. citations | 5 avg, IF | 6.18 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 150 | Three-dimensional Langevin dynamics of N atom scattering from N-covered Ag(1 1 1). *Chemical Physics*, **2022**, 560, 111557 | 2.3 | |
| 149 | Assessing density functionals for describing methane dissociative chemisorption on Pt(110)-(2×1) surface. *Chinese Journal of Chemical Physics*, **2021**, 34, 883-895 | 0.9 | 1 |
| 148 | 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). *Journal of Physical Chemistry C*, **2021**, 125, 8993-9010 | 3.8 | 3 |
| 147 | Highly Efficient Activation of HCl Dissociation on Au(111) via Rotational Preexcitation. *Journal of Physical Chemistry Letters*, **2021**, 12, 7252-7260 | 6.4 | 0 |
| 146 | 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). *Physical Chemistry Chemical Physics*, **2021**, 23, 7875-7901 | 3.6 | 6 |
| 145 | Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. *Physical Chemistry Chemical Physics*, **2021**, 23, 8962-9048 | 3.6 | 26 |
| 144 | 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. *Journal of Physical Chemistry Letters*, **2020**, 11, 10552-10560 | 6.4 | 20 |
| 143 | Closing the Gap Between Experiment and Theory: Reactive Scattering of HCl from Au(111). *Journal of Physical Chemistry C*, **2020**, 124, 15944-15960 | 3.8 | 12 |
| 142 | Quantum Monte Carlo calculations on dissociative chemisorption of H + Al(110): Minimum barrier heights and their comparison to DFT values. *Journal of Chemical Physics*, **2020**, 153, 224701 | 3.9 | 8 |
| 141 | Dynamical Study of the Dissociative Chemisorption of CHD on Pd(111). *Journal of Physical Chemistry C*, **2019**, 123, 24013-24023 | 3.8 | 8 |
| 140 | Specific Reaction Parameter Density Functional Based on the Meta-Generalized Gradient Approximation: Application to H + Cu(111) and H + Ag(111). *Journal of Physical Chemistry A*, **2019**, 123, 5395-5406 | 2.8 | 20 |
| 139 | CHD3 Dissociation on the Kinked Pt(210) Surface: A Comparison of Experiment and Theory. *Journal of Physical Chemistry C*, **2019**, 123, 14530-14539 | 3.8 | 10 |
| 138 | Orbital-Dependent Electronic Friction Significantly Affects the Description of Reactive Scattering of N from Ru(0001). *Journal of Physical Chemistry Letters*, **2019**, 10, 2957-2962 | 6.4 | 33 |
| 137 | Transferability of the SRP32-vdW specific reaction parameter functional to CHD dissociation on Pt(110)-(2×1). *Journal of Chemical Physics*, **2019**, 150, 124702 | 3.9 | 14 |
| 136 | Assessment of Two Problems of Specific Reaction Parameter Density Functional Theory: Sticking and Diffraction of H on Pt(111). *Journal of Physical Chemistry C*, **2019**, 123, 10406-10418 | 3.8 | 9 |
| 135 | Accurate Probabilities for Highly Activated Reaction of Polyatomic Molecules on Surfaces Using a High-Dimensional Neural Network Potential: CHD + Cu(111). *Journal of Physical Chemistry Letters*, **2019**, 10, 1763-1768 | 6.4 | 42 |
| 134 | Quantum Dynamics of Dissociative Chemisorption of H on the Stepped Cu(211) Surface. *Journal of Physical Chemistry C*, **2019**, 123, 23049-23063 | 3.8 | 15 |

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| 133 | Toward a Specific Reaction Parameter Density Functional for H2 + Ni(111): Comparison of Theory with Molecular Beam Sticking Experiments. *Journal of Physical Chemistry C*, **2019**, 123, 20420-20433 | 3.8 | 9 |
| 132 | Curious Mechanism of the Dissociative Chemisorption of Ammonia on Ru(0001). *Journal of Physical Chemistry C*, **2019**, 123, 28291-28300 | 3.8 | 9 |
| 131 | Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2019**, 123, 2287-2299 | 3.8 | 21 |
| 130 | Transferability of the Specific Reaction Parameter Density Functional for H + Pt(111) to H + Pt(211). *Journal of Physical Chemistry C*, **2019**, 123, 2973-2986 | 3.8 | 16 |
| 129 | An AIMD study of dissociative chemisorption of methanol on Cu(111) with implications for formaldehyde formation. *Journal of Chemical Physics*, **2019**, 150, 024706 | 3.9 | 8 |
| 128 | Anomalous Dependence of the Reactivity on the Presence of Steps: Dissociation of D on Cu(211). *Journal of Physical Chemistry Letters*, **2018**, 9, 170-175 | 6.4 | 23 |
| 127 | Incident Angle Dependence of CHD Dissociation on the Stepped Pt(211) Surface. *Journal of Physical Chemistry C*, **2018**, 122, 19652-19660 | 3.8 | 15 |
| 126 | Density functional embedding for periodic and nonperiodic diffusion Monte Carlo calculations. *Physical Review B*, **2018**, 98, | 3.3 | 7 |
| 125 | HOD on Ni(111): molecular dynamics prediction of molecular beam experiments. *Journal of Chemical Physics*, **2018**, 149, 244706 | 3.9 | 11 |
| 124 | Dissociation of CHD on Cu(111), Cu(211), and single atom alloys of Cu(111). *Journal of Chemical Physics*, **2018**, 149, 224701 | 3.9 | 12 |
| 123 | Analysis of Energy Dissipation Channels in a Benchmark System of Activated Dissociation: N on Ru(0001). *Journal of Physical Chemistry C*, **2018**, 122, 23470-23480 | 3.8 | 11 |
| 122 | Test of the Transferability of the Specific Reaction Parameter Functional for H + Cu(111) to D + Ag(111). *Journal of Physical Chemistry C*, **2018**, 122, 22939-22952 | 3.8 | 9 |
| 121 | CHD dissociation on Pt(111): A comparison of the reaction dynamics based on the PBE functional and on a specific reaction parameter functional. *Journal of Chemical Physics*, **2018**, 149, 044701 | 3.9 | 14 |
| 120 | Methane on a stepped surface: Dynamical insights on the dissociation of CHD on Pt(111) and Pt(211). *Journal of Chemical Physics*, **2018**, 149, 094701 | 3.9 | 12 |
| 119 | Chemically accurate simulation of dissociative chemisorption of D2 on Pt(1 1 1). *Chemical Physics Letters*, **2017**, 683, 329-335 | 2.5 | 33 |
| 118 | A general method for controlling and resolving rotational orientation of molecules in molecule-surface collisions. *Nature Communications*, **2017**, 8, 15357 | 17.4 | 26 |
| 117 | Accurate Neural Network Description of Surface Phonons in Reactive Gas-Surface Dynamics: N + Ru(0001). *Journal of Physical Chemistry Letters*, **2017**, 8, 2131-2136 | 6.4 | 103 |
| 116 | Exploring surface landscapes with molecules: rotationally induced diffraction of H on LiF(001) under fast grazing incidence conditions. *Physical Chemistry Chemical Physics*, **2017**, 19, 16317-16322 | 3.6 | 4 |

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| 115 | Vibrational Excitation of H Scattering from Cu(111): Effects of Surface Temperature and of Allowing Energy Exchange with the Surface. *Journal of Physical Chemistry C*, **2017**, 121, 13617-13633 | 3.8 | 22 |
| 114 | Quantum Monte Carlo Calculations on a Benchmark Molecule-Metal Surface Reaction: H + Cu(111). *Journal of Chemical Theory and Computation*, **2017**, 13, 3208-3219 | 6.4 | 24 |
| 113 | Surface Reaction Barriometry: Methane Dissociation on Flat and Stepped Transition-Metal Surfaces. *Journal of Physical Chemistry Letters*, **2017**, 8, 4177-4182 | 6.4 | 64 |
| 112 | SBH10: A Benchmark Database of Barrier Heights on Transition Metal Surfaces. *Journal of Physical Chemistry C*, **2017**, 121, 19807-19815 | 3.8 | 67 |
| 111 | H2/LiF(001) diffractive scattering under fast grazing incidence using a DFT-based potential energy surface. *Physical Review B*, **2017**, 96, | 3.3 | 3 |
| 110 | Dissociative chemisorption of methane on Ni(111) using a chemically accurate fifteen dimensional potential energy surface. *Physical Chemistry Chemical Physics*, **2017**, 19, 30540-30550 | 3.6 | 36 |
| 109 | Possible effect of static surface disorder on diffractive scattering of H from Ru(0001): Comparison between theory and experiment. *Journal of Chemical Physics*, **2017**, 147, 244705 | 3.9 | 7 |
| 108 | Quantum and classical dynamics of reactive scattering of H2 from metal surfaces. *Chemical Society Reviews*, **2016**, 45, 3658-700 | 58.5 | 116 |
| 107 | Enigmatic HCl + Au(111) Reaction: A Puzzle for Theory and Experiment. *Journal of Physical Chemistry C*, **2016**, 120, 25760-25779 | 3.8 | 40 |
| 106 | Diffusion Monte Carlo for Accurate Dissociation Energies of 3d Transition Metal Containing Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 2583-97 | 6.4 | 37 |
| 105 | Chemically Accurate Simulation of a Polyatomic Molecule-Metal Surface Reaction. *Journal of Physical Chemistry Letters*, **2016**, 7, 2402-6 | 6.4 | 93 |
| 104 | Rotational effects on the dissociation dynamics of CHD3 on Pt(111). *Physical Chemistry Chemical Physics*, **2016**, 18, 8174-85 | 3.6 | 22 |
| 103 | Modeling surface motion effects in N2 dissociation on W(110): Ab initio molecular dynamics calculations and generalized Langevin oscillator model. *Journal of Chemical Physics*, **2016**, 144, 244708 | 3.9 | 18 |
| 102 | Methane dissociation on Pt(111): Searching for a specific reaction parameter density functional. *Journal of Chemical Physics*, **2016**, 144, 044702 | 3.9 | 45 |
| 101 | Application of van der Waals functionals to the calculation of dissociative adsorption of N2 on W(110) for static and dynamic systems. *Journal of Chemical Physics*, **2016**, 144, 084702 | 3.9 | 12 |
| 100 | Dynamics of H dissociation on the close-packed (111) surface of the noblest metal: H + Au(111). *Journal of Chemical Physics*, **2016**, 145, 144701 | 3.9 | 19 |
| 99 | An ab initio molecular dynamics study of D2 dissociation on CO-precovered Ru(0001). *Physical Chemistry Chemical Physics*, **2016**, 18, 21190-201 | 3.6 | 3 |
| 98 | Toward a Database of Chemically Accurate Barrier Heights for Reactions of Molecules with Metal Surfaces. *Journal of Physical Chemistry Letters*, **2015**, 6, 4106-14 | 6.4 | 61 |

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| 97 | Performance of a Non-Local van der Waals Density Functional on the Dissociation of H2 on Metal Surfaces. *Journal of Physical Chemistry A*, **2015**, 119, 12146-58 | 2.8 | 37 |
| 96 | N2 dissociation on W(110): An ab initio molecular dynamics study on the effect of phonons. *Journal of Chemical Physics*, **2015**, 142, 104702 | 3.9 | 17 |
| 95 | Dissociative chemisorption of methane on metal surfaces: tests of dynamical assumptions using quantum models and ab initio molecular dynamics. *Journal of Chemical Physics*, **2014**, 141, 054102 | 3.9 | 75 |
| 94 | Ab Initio Molecular Dynamics Calculations versus Quantum-State-Resolved Experiments on CHD3 + Pt(111): New Insights into a Prototypical Gas-Surface Reaction. *Journal of Physical Chemistry Letters* , **2014**, 5, 1294-9 | 6.4 | 112 |
| 93 | The effect of the exchange-correlation functional on H2 dissociation on Ru(0001). *Journal of Chemical Physics*, **2014**, 140, 084702 | 3.9 | 51 |
| 92 | Dissociation and recombination of D□n Cu(111): ab initio molecular dynamics calculations and improved analysis of desorption experiments. *Journal of Chemical Physics*, **2014**, 141, 124705 | 3.9 | 30 |
| 91 | Electronic friction dominates hydrogen hot-atom relaxation on Pd(100). *Physical Review Letters*, **2014**, 112, 103203 | 7.4 | 97 |
| 90 | Ab initio molecular dynamics calculations on scattering of hyperthermal H atoms from Cu(111) and Au(111). *Journal of Chemical Physics*, **2014**, 141, 054705 | 3.9 | 37 |
| 89 | Adiabatic Energy Loss in Hyperthermal H Atom Collisions with Cu and Au: A Basis for Testing the Importance of Nonadiabatic Energy Loss. *Journal of Physical Chemistry Letters*, **2013**, 4, 3735-3740 | 6.4 | 42 |
| 88 | 7D Quantum Dynamics of H2 Scattering from Cu(111): The Accuracy of the Phonon Sudden Approximationy. *Zeitschrift Fur Physikalische Chemie*, **2013**, 130617035227002 | 3.1 | 13 |
| 87 | 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. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227, | 3.1 | 16 |
| 86 | Surface Temperature Effects on Dissociative Chemisorption of H2 on Cu(100). *Journal of Physical Chemistry C*, **2013**, 117, 8851-8863 | 3.8 | 27 |
| 85 | Effect of Transition Metal Dopants on Initial Mass Transport in the Dehydrogenation of NaAlH4: Density Functional Theory Study. *Journal of Physical Chemistry C*, **2013**, 117, 3-14 | 3.8 | 18 |
| 84 | Thermal lattice expansion effect on reactive scattering of H2 from Cu(111) at T(s) = 925 K. *Journal of Physical Chemistry A*, **2013**, 117, 8770-81 | 2.8 | 43 |
| 83 | Towards a specific reaction parameter density functional for reactive scattering of H2 from Pd(111). *Journal of Chemical Physics*, **2013**, 139, 244707 | 3.9 | 14 |
| 82 | Reactive scattering of H2 from Cu(100): comparison of dynamics calculations based on the specific reaction parameter approach to density functional theory with experiment. *Journal of Chemical Physics*, **2013**, 138, 044708 | 3.9 | 66 |
| 81 | Dynamics of H2 dissociation on the 1/2 ML c(2 □2)-Ti/Al(100) surface. *Physical Chemistry Chemical Physics*, **2012**, 14, 3234-47 | 3.6 | 12 |
| 80 | H2 Diffraction from a Strained Pseudomorphic Monolayer of Cu Deposited on Ru(0001). *Journal of Physical Chemistry C*, **2012**, 116, 13671-13678 | 3.8 | 15 |

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| 79 | Towards chemically accurate simulation of molecule-surface reactions. *Physical Chemistry Chemical Physics*, **2012**, 14, 14966-81 | 3.6 | 73 |
| 78 | Theoretical Investigation of Two H2 Molecules Inside the Cages of the Structure H Clathrate Hydrate. *Journal of Physical Chemistry C*, **2012**, 116, 21664-21672 | 3.8 | 20 |
| 77 | Effect of surface motion on the rotational quadrupole alignment parameter of D2 reacting on Cu(111). *Physical Review Letters*, **2012**, 108, 236104 | 7.4 | 89 |
| 76 | Chebyshev high-dimensional model representation (Chebyshev-HDMR) potentials: application to reactive scattering of H2 from Pt(111) and Cu(111) surfaces. *Physical Chemistry Chemical Physics*, **2012**, 14, 8628-43 | 3.6 | 16 |
| 75 | Vibrational deexcitation and rotational excitation of H2 and D2 scattered from Cu(111): adiabatic versus non-adiabatic dynamics. *Journal of Chemical Physics*, **2012**, 137, 064707 | 3.9 | 40 |
| 74 | Diffractive and reactive scattering of H2 from Ru(0001): experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2011**, 13, 8583-97 | 3.6 | 32 |
| 73 | Hydrogen dissociation on Cu(111): the influence of lattice motion. Part I. *Physical Chemistry Chemical Physics*, **2011**, 13, 4552-61 | 3.6 | 50 |
| 72 | Six-dimensional quasiclassical and quantum dynamics of H2 dissociation on the c(2 ⊠2)-Ti/Al(100) surface. *Journal of Chemical Physics*, **2011**, 134, 114708 | 3.9 | 13 |
| 71 | A theoretical study of H(2) dissociation on (sq.rt(3) x sq.rt(3))R30 degrees CO/Ru(0001). *Journal of Chemical Physics*, **2010**, 132, 144704 | 3.9 | 4 |
| 70 | Apparent failure of the Born-Oppenheimer static surface model for vibrational excitation of molecular hydrogen on copper. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 20881-6 | 11.5 | 45 |
| 69 | Quantum dynamics of dissociative chemisorption of CH(4) on Ni(111): Influence of the bending vibration. *Journal of Chemical Physics*, **2010**, 133, 144308 | 3.9 | 64 |
| 68 | Dynamics on Six-Dimensional Potential Energy Surfaces for H2/Cu(111): Corrugation Reducing Procedure versus Modified Shepard Interpolation Method and PW91 versus RPBE. *Journal of Physical Chemistry C*, **2010**, 114, 11192-11201 | 3.8 | 47 |
| 67 | Molecular dynamics simulations of the ice temperature dependence of water ice photodesorption. *Journal of Chemical Physics*, **2010**, 132, 184510 | 3.9 | 56 |
| 66 | Six-dimensional dynamics study of reactive and non reactive scattering of H(2) from Cu(111) using a chemically accurate potential energy surface. *Physical Chemistry Chemical Physics*, **2010**, 12, 6499-519 | 3.6 | 82 |
| 65 | Dynamics of dissociative adsorption of hydrogen on a CO-precovered Ru(0001) surface: a comparison of theoretical and experimental results. *Physical Chemistry Chemical Physics*, **2010**, 12, 1331-40 | 3.6 | 17 |
| 64 | A Theoretical Study of H2 Reacting on Ti/Al(100) Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 11027-11034 | 3.8 | 17 |
| 63 | Chemically accurate simulation of a prototypical surface reaction: H2 dissociation on Cu(111). *Science*, **2009**, 326, 832-4 | 33.3 | 282 |
| 62 | Frontiers in surface scattering simulations. *Science*, **2008**, 321, 794-7 | 33.3 | 101 |

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| 61 | Using n-mode potentials for reactive scattering: Application to the 6D H2 + Pt(1 1 1) problem. *Chemical Physics Letters*, **2007**, 440, 334-340 | 2.5 | 14 |
| 60 | Dissociative chemisorption of H2 on the Cu(110) surface: a quantum and quasiclassical dynamical study. *Journal of Chemical Physics*, **2007**, 127, 164722 | 3.9 | 36 |
| 59 | Theoretical Study of Stable, Defect-Free (TiO2)nNanoparticles withn= 10□16. *Journal of Physical Chemistry C*, **2007**, 111, 16808-16817 | 3.8 | 106 |
| 58 | Multiconfiguration time-dependent Hartree method applied to molecular dissociation on surfaces: H2 + Pt(111). *Journal of Chemical Physics*, **2006**, 124, 74706 | 3.9 | 22 |
| 57 | Multidimensional effects on dissociation of N2 on Ru(0001). *Physical Review Letters*, **2006**, 96, 096102 | 7.4 | 85 |
| 56 | Quantum dynamical study of the H2 and D2 dissociative adsorption and diffraction from the NiAl (110) alloy surface. *Physical Review B*, **2006**, 73, | 3.3 | 24 |
| 55 | Reactive and nonreactive scattering of H2 from a metal surface is electronically adiabatic. *Science*, **2006**, 312, 86-9 | 33.3 | 173 |
| 54 | Predicting catalysis: understanding ammonia synthesis from first-principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 17719-35 | 3.4 | 168 |
| 53 | Reactive and nonreactive scattering of N2 from Ru(0001): a six-dimensional adiabatic study. *Journal of Chemical Physics*, **2006**, 125, 114706 | 3.9 | 40 |
| 52 | Identifying spectator bonds in modeling reactions: OH+CO->H+CO2. *Chemical Physics Letters*, **2006**, 417, 43-47 | 2.5 | 15 |
| 51 | The HD isotope effect in the stability of lithium alanate. *Chemical Physics Letters*, **2006**, 423, 102-105 | 2.5 | 21 |
| 50 | Quasiharmonic approximation applied to LiBH4 and its decomposition products. *Physical Review B*, **2006**, 73, | 3.3 | 44 |
| 49 | A classical dynamics method for H2 diffraction from metal surfaces. *Journal of Chemical Physics*, **2005**, 122, 154706 | 3.9 | 27 |
| 48 | Theory of Molecular Scattering from and Photochemistry at Ice Surfaces. *Proceedings of the International Astronomical Union*, **2005**, 1, 427 | 0.1 | 3 |
| 47 | Theoretical calculation of the energy of formation of LiBH4. *Chemical Physics Letters*, **2005**, 405, 73-78 | 2.5 | 79 |
| 46 | Quantum and classical dynamics of H2 scattering from Pd(111) at off-normal incidence. *Physical Review B*, **2005**, 72, | 3.3 | 22 |
| 45 | Six-dimensional quantum dynamics of (v=0,j=0)D2 and of (v=1,j=0)H2 scattering from Cu111. *Journal of Chemical Physics*, **2005**, 122, 214709 | 3.9 | 27 |
| 44 | Six-dimensional quantum dynamics of dissociative chemisorption of H2 on Ru(0001). *Journal of Chemical Physics*, **2005**, 122, 44701 | 3.9 | 59 |

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| 43 | SIX-DIMENSIONAL DYNAMICS OF DISSOCIATIVE CHEMISORPTION OF H2 ON METAL SURFACES. *Journal of Theoretical and Computational Chemistry*, **2005**, 04, 493-581 | 1.8 | 76 |
| 42 | In-plane and out-of-plane diffraction of H(2) from metal surfaces. *Physical Review Letters*, **2004**, 93, 246104 | 7.4 | 68 |
| 41 | Role of CO vibration in the complex-forming OH+CO->H+CO2 reaction. *Physical Review A*, **2004**, 70, | 2.6 | 21 |
| 40 | Application of the modified Shepard interpolation method to the determination of the potential energy surface for a molecule-surface reaction: H2 + Pt(111). *Journal of Chemical Physics*, **2004**, 120, 2392-404 | 3.9 | 81 |
| 39 | New results for the OH (nu = 0,j = 0) + CO (nu = 0,j = 0) --> H + CO2 reaction: Five- and full-dimensional quantum dynamical study on several potential energy surfaces. *Journal of Chemical Physics*, **2004**, 120, 4263-72 | 3.9 | 48 |
| 38 | Reactive scattering of H2 from Cu(100): six-dimensional quantum dynamics results for reaction and scattering obtained with a new, accurately fitted potential-energy surface. *Journal of Chemical Physics*, **2004**, 121, 11379-87 | 3.9 | 23 |
| 37 | Efficient penetration of the basal plane (0001) face of ice Ih by HF at Ts=150 K: dependence on incidence energy, incidence angle, and rotational energy. *Journal of Chemical Physics*, **2004**, 120, 11796-803 | 3.9 | 7 |
| 36 | Performance and application of a symmetry adapted pseudo spectral method for scattering of a diatomic molecule from a square surface: H2 + Cu(1 0 0). *Chemical Physics*, **2004**, 304, 59-77 | 2.3 | 7 |
| 35 | The dependence of dissociative chemisorption of H2 on Pd(1 1 1) on H2 rotation: a six-dimensional quantum dynamics study. *Chemical Physics Letters*, **2004**, 393, 166-172 | 2.5 | 6 |
| 34 | Theoretical Reaction Dynamics Study of the Effect of Vibrational Excitation of CO on the OH + CO -> H + CO2Reaction *Journal of Physical Chemistry A*, **2004**, 108, 8672-8681 | 2.8 | 27 |
| 33 | Multi-dimensional potential energy surface determination by modified Shepard interpolation for a molecule surface reaction: H2 + Pt(1 1 1). *Chemical Physics Letters*, **2003**, 376, 566-575 | 2.5 | 54 |
| 32 | Predictions on the effect of initial molecular orientation and rotation on penetration of the (0001) face of hexagonal ice by HCl. *Chemical Physics Letters*, **2003**, 376, 581-587 | 2.5 | 5 |
| 31 | Rotational effects in dissociation of H2 on Pd(111): Quantum and classical study. *Journal of Chemical Physics*, **2003**, 119, 12553-12562 | 3.9 | 48 |
| 30 | Diffractive and reactive scattering of (v=0, j=0) HD from Pt(111): Six-dimensional quantum dynamics compared with experiment. *Journal of Chemical Physics*, **2003**, 118, 4190-4197 | 3.9 | 30 |
| 29 | Full-dimensional quantal initial state-selected reaction probabilities (J=0) for the reaction OH(v=0,j=0)+CO(v=0,j=0)->CO2+H. *Chemical Physics Letters*, **2002**, 352, 281-287 | 2.5 | 25 |
| 28 | Six-dimensional quantum dynamics of scattering of (v=0,j=0) H2 and D2 from Cu(111): test of two LEPS potential energy surfaces. *Chemical Physics Letters*, **2002**, 360, 390-399 | 2.5 | 47 |
| 27 | Converged five-dimensional quantum calculations for OH+CO->H+CO2. *Journal of Chemical Physics*, **2002**, 116, 4184-4191 | 3.9 | 16 |
| 26 | Theoretical rate constants for the OH+CO->H+CO2 reaction using variational transition state theory on analytical potential energy surfaces. *Journal of Chemical Physics*, **2002**, 117, 8736-8744 | 3.9 | 27 |

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| 25 | Reactive and diffractive scattering of H2 from Pt(111) studied using a six-dimensional wave packet method. *Journal of Chemical Physics*, **2002**, 117, 5885-5898 | 3.9 | 107 |
| 24 | Dissociative and diffractive scattering of H2 from Pt(111): A four-dimensional quantum dynamics study. *Journal of Chemical Physics*, **2002**, 116, 9435-9448 | 3.9 | 28 |
| 23 | Signatures of site-specific reaction of H2 on Cu(100). *Journal of Chemical Physics*, **2002**, 117, 6673-6687 | 3.9 | 33 |
| 22 | Quantum theory of dissociative chemisorption on metal surfaces. *Accounts of Chemical Research*, **2002**, 35, 193-200 | 24.3 | 154 |
| 21 | Constructing accurate potential energy surfaces for a diatomic molecule interacting with a solid surface: H2+Pt(111) and H2+Cu(100). *Journal of Chemical Physics*, **2002**, 116, 3841-3855 | 3.9 | 127 |
| 20 | Six-dimensional quantum dynamics of scattering of (v=0, j=0) H2 from Pt(111): comparison to experiment and to classical dynamics results. *Chemical Physics Letters*, **2001**, 347, 277-284 | 2.5 | 63 |
| 19 | Sticking of HCl to ice at hyperthermal energies: Dependence on incidence energy, incidence angle, and surface temperature. *Journal of Chemical Physics*, **2001**, 115, 482-491 | 3.9 | 26 |
| 18 | Rovibrationally inelastic scattering of (v=1, j=1) H2 from Cu(100): Experiment and theory. *Journal of Chemical Physics*, **2001**, 114, 495 | 3.9 | 56 |
| 17 | Molecular knife throwing: aiming for dissociation at specific surface sites through state-selection. *Chemical Physics Letters*, **2000**, 328, 317-324 | 2.5 | 31 |
| 16 | The effect of corrugation on the quantum dynamics of dissociative and diffractive scattering of H2 from Pt(111). *Journal of Chemical Physics*, **2000**, 113, 8300-8312 | 3.9 | 31 |
| 15 | Quantum dynamics of the dissociation of H2 on Cu(100): dependence of the site-reactivity on initial rovibrational state. *Faraday Discussions*, **2000**, 109-32; discussion 161-89 | 3.6 | 33 |
| 14 | Atomic and molecular hydrogen interacting with Pt(111). *Journal of Chemical Physics*, **1999**, 111, 11155-11163 | 3.9 | 176 |
| 13 | Rotational Effects on Vibrational Excitation of H2 on Cu(100). *Physical Review Letters*, **1999**, 82, 1410-1413 | 7.4 | 30 |
| 12 | A classical study of rotational effects in dissociation of H2 on Cu(100). *Physical Chemistry Chemical Physics*, **1999**, 1, 1359-1374 | 3.6 | 28 |
| 11 | Accuracy of trajectory methods for activated adsorption of H2 on Cu(100). *Chemical Physics Letters*, **1998**, 296, 515-520 | 2.5 | 30 |
| 10 | Six-dimensional quantum dynamics of dissociative chemisorption of H2 on Cu(100). *Journal of Chemical Physics*, **1997**, 107, 3309-3323 | 3.9 | 68 |
| 9 | The influence of surface motion on the direct subsurface absorption of H2 on Pd(111). *Journal of Chemical Physics*, **1997**, 107, 10652-10661 | 3.9 | 36 |
| 8 | Six-Dimensional Quantum Dynamics of Dissociative Chemisorption of ( v=0, j=0) H2 on Cu(100). *Physical Review Letters*, **1997**, 78, 3583-3586 | 7.4 | 109 |

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| 7 | An analytical six-dimensional potential energy surface for dissociation of molecular hydrogen on Cu(100). *Journal of Chemical Physics*, **1996**, 104, 7344-7358 | 3.9 | 106 |
| 6 | Competition between vibrational excitation and dissociation in collisions of H2 with Cu(100). *Physical Review B*, **1996**, 53, 10397-10401 | 3.3 | 49 |
| 5 | Performance of close-coupled wave packet methods for molecule-corrugated surface scattering. *Journal of Chemical Physics*, **1995**, 103, 5121-5136 | 3.9 | 29 |
| 4 | Dissociation of H2 on Cu(100): Dynamics on a new two-dimensional potential energy surface. *Journal of Chemical Physics*, **1995**, 102, 3873-3883 | 3.9 | 63 |
| 3 | Application of an efficient asymptotic analysis method to molecule-surface scattering. *Journal of Chemical Physics*, **1995**, 103, 1216-1225 | 3.9 | 47 |
| 2 | Performance of a fully close-coupled wave packet method for the H2+LiF(001) model problem. *Journal of Chemical Physics*, **1995**, 102, 5512-5524 | 3.9 | 30 |
| 1 | Calculations on rotationally and diffractionally inelastic molecule-surface scattering for arbitrary angles of incidence: A new wave packet technique. *Journal of Chemical Physics*, **1994**, 101, 805-813 | 3.9 | 19 |