# Daiqian Xie

## List of Publications by Year in Descending Order



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| 216 papers | 4,556 citations | 37 h-index | 53 g-index |
| 227 ext. papers | 4,981 ext. citations | 5.2 avg, IF | 5.82 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 216 | Adiabatic potential energy surfaces and photodissociation mechanisms for highly excited states of H2O. *Chinese Journal of Chemical Physics*, **2022**, 35, 104-116 | 0.9 | |
| 215 | Reaction Pathway Control via Reactant Vibrational Excitation and Impact on Product Vibrational Distributions: The O + HO -> OH + O Atmospheric Reaction.. *Journal of Physical Chemistry Letters*, **2022**, 1872-1878 | 6.4 | 0 |
| 214 | Stereodynamical Control of Cold Collisions of Polyatomic Molecules with Atoms.. *Journal of Physical Chemistry Letters*, **2022**, 1777-1784 | 6.4 | 1 |
| 213 | Vibrationally excited molecular hydrogen production from the water photochemistry. *Nature Communications*, **2021**, 12, 6303 | 17.4 | 3 |
| 212 | Quantum Dynamics of Rotational Energy Transfer Processes for N-HF and N-DF Systems. *Journal of Physical Chemistry A*, **2021**, 125, 349-355 | 2.8 | 0 |
| 211 | Quantum dynamics of the energy transfer for vibrationally excited HF (v = 7) colliding with D (v = 0): Theory assessing experiment. *Journal of Chemical Physics*, **2021**, 154, 114303 | 3.9 | 0 |
| 210 | Interaction-Asymptotic Region Decomposition Method for a Triatomic Reactive Scattering with Symmetry Adoption. *Journal of Physical Chemistry A*, **2021**, 125, 2460-2471 | 2.8 | 1 |
| 209 | Three body photodissociation of the water molecule and its implications for prebiotic oxygen production. *Nature Communications*, **2021**, 12, 2476 | 17.4 | 6 |
| 208 | Precision test of statistical dynamics with state-to-state ultracold chemistry. *Nature*, **2021**, 593, 379-384 | 50.4 | 21 |
| 207 | Strong isotope effect in the VUV photodissociation of HOD: A possible origin of D/H isotope heterogeneity in the solar nebula. *Science Advances*, **2021**, 7, | 14.3 | 2 |
| 206 | Rotational Modulation of ?-State Photodissociation of HCO via Renner-Teller Nonadiabatic Transitions. *Journal of Physical Chemistry Letters*, **2021**, 12, 6582-6588 | 6.4 | 1 |
| 205 | Full-Dimensional Global Potential Energy Surface for the KRb + KRb -> KRb* -> K + Rb Reaction with Accurate Long-Range Interactions and Quantum Statistical Calculation of the Product State Distribution under Ultracold Conditions. *Journal of Physical Chemistry A*, **2021**, 125, 6198-6206 | 2.8 | 2 |
| 204 | Insights into the Formation of Hydroxyl Radicals with Nonthermal Vibrational Excitation in the Meinel Airglow. *Journal of Physical Chemistry Letters*, **2021**, 12, 1822-1828 | 6.4 | 2 |
| 203 | Interaction-Asymptotic Region Decomposition Method for an Insertion Reaction: Application to the S(D) + H Reaction. *Journal of Physical Chemistry A*, **2021**, 125, 2007-2018 | 2.8 | 2 |
| 202 | Spontaneous Polarity Flipping in a 2D Heterobilayer Induced by Fluctuating Interfacial Carrier Flows. *Nano Letters*, **2021**, 21, 6773-6780 | 11.5 | 1 |
| 201 | A Time-Independent Quantum Approach to Ro-vibrationally Inelastic Scattering between Atoms and Triatomic Molecules. *Journal of Physical Chemistry A*, **2021**, 125, 6864-6871 | 2.8 | 2 |
| 200 | A full-dimensional ab initio intermolecular potential energy surface and rovibrational spectra for OC-HF and OC-DF. *Journal of Chemical Physics*, **2021**, 155, 084302 | 3.9 | 0 |

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| 199 | Theoretical H + O rate coefficients from ring polymer molecular dynamics on an accurate global potential energy surface: assessing experimental uncertainties. *Physical Chemistry Chemical Physics*, **2021**, 23, 3300-3310 | 3.6 | 3 |
| 198 | Nonadiabatic Electronic Energy Transfer in the Chemical Oxygen-Iodine Laser: Powered by Derivative Coupling or Spin-Orbit Coupling?. *Journal of Physical Chemistry Letters*, **2020**, 11, 4768-4773 | 6.4 | 7 |
| 197 | A theoretical study on quantum dynamics of energy transfer for HF colliding with D2. *European Physical Journal D*, **2020**, 74, 1 | 1.3 | 2 |
| 196 | A Global Full-Dimensional Potential Energy Surface for the KRb Complex and Its Lifetime. *Journal of Physical Chemistry Letters*, **2020**, 11, 2605-2610 | 6.4 | 12 |
| 195 | Statistical quantum mechanical approach to diatom-diatom capture dynamics and application to ultracold KRb + KRb reaction. *Journal of Chemical Physics*, **2020**, 152, 241103 | 3.9 | 10 |
| 194 | A full-dimensional ab initio intermolecular potential energy surface and ro-vibrational spectra for N-HF and N-DF. *Journal of Chemical Physics*, **2020**, 152, 084304 | 3.9 | 1 |
| 193 | Mechanisms of Oxygen Passivation on Surface Defects in MAPbI3 Revealed by First-Principles Study. *Journal of Physical Chemistry C*, **2020**, 124, 3731-3737 | 3.8 | 4 |
| 192 | Cobalt/zinc dual-sites coordinated with nitrogen in nanofibers enabling efficient and durable oxygen reduction reaction in acidic fuel cells. *Journal of Materials Chemistry A*, **2020**, 8, 3686-3691 | 13 | 42 |
| 191 | Mode Specificity in the OH + HO -> HO + O Reaction: Enhancement of Reactivity by Exciting a Spectator Mode. *Journal of the American Chemical Society*, **2020**, 142, 3331-3335 | 16.4 | 24 |
| 190 | Dynamics Studies of O2 Collision on Pt(111) Using a Global Potential Energy Surface. *Journal of Physical Chemistry C*, **2020**, 124, 10573-10583 | 3.8 | 4 |
| 189 | Insights into the Mechanism of Nonadiabatic Photodissociation from Product Vibrational Distributions. The Remarkable Case of Phenol. *Journal of Physical Chemistry Letters*, **2020**, 11, 191-198 | 6.4 | 15 |
| 188 | State-to-state chemical kinetic mechanism for HF chemical lasers. *Combustion Theory and Modelling*, **2020**, 24, 129-141 | 1.5 | 2 |
| 187 | Water Photolysis and Its Contributions to the Hydroxyl Dayglow Emissions in the Atmospheres of Earth and Mars. *Journal of Physical Chemistry Letters*, **2020**, 11, 9086-9092 | 6.4 | 9 |
| 186 | Probing the Potential Energy Surfaces of BrCN by Dissociative Electron Attachment. *Journal of Physical Chemistry Letters*, **2020**, 11, 9110-9116 | 6.4 | 1 |
| 185 | Theoretical Investigations of Rate Coefficients for H + O and HO + O Reactions on a Full-Dimensional Potential Energy Surface. *Journal of Physical Chemistry A*, **2020**, 124, 6427-6437 | 2.8 | 12 |
| 184 | Origin of the "odd" behavior in the ultraviolet photochemistry of ozone. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 21065-21069 | 11.5 | 5 |
| 183 | Advances and New Challenges to Bimolecular Reaction Dynamics Theory. *Journal of Physical Chemistry Letters*, **2020**, 11, 8844-8860 | 6.4 | 27 |
| 182 | Electronically Excited OH Super-rotors from Water Photodissociation by Using Vacuum Ultraviolet Free-Electron Laser Pulses. *Journal of Physical Chemistry Letters*, **2020**, 11, 7617-7623 | 6.4 | 9 |

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| 181 | Computational determination of binding modes of 2-acetoxyphenylhept-2-ynyl sulfide to cyclooxygenase-2. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3648-3658 | 3.6 | 1 |
| 180 | Aqueous Self-Assembly of Amphiphilic Cyclic Brush Block Copolymers as Asymmetry-Tunable Building Blocks. *Macromolecules*, **2019**, 52, 7042-7051 | 5.5 | 9 |
| 179 | Dissection of the multichannel reaction of acetylene with atomic oxygen: from the global potential energy surface to rate coefficients and branching dynamics. *Physical Chemistry Chemical Physics*, **2019**, 21, 1408-1416 | 3.6 | 3 |
| 178 | Molecular insight into chymotrypsin inhibitor 2 resisting proteolytic degradation. *Physical Chemistry Chemical Physics*, **2019**, 21, 5049-5058 | 3.6 | 3 |
| 177 | First-principles dynamics of collisional intersystem crossing: resonance enhanced quenching of C(D) by N. *Physical Chemistry Chemical Physics*, **2019**, 21, 8645-8653 | 3.6 | 6 |
| 176 | Linking inhibitor motions to proteolytic stability of sunflower trypsin inhibitor-1.. *RSC Advances*, **2019**, 9, 13776-13786 | 3.7 | 2 |
| 175 | An ab initio based full-dimensional potential energy surface for OH + O? HO and low-lying vibrational levels of HO. *Physical Chemistry Chemical Physics*, **2019**, 21, 13766-13775 | 3.6 | 8 |
| 174 | Anomalous kinetics of the reaction between OH and HO on an accurate triplet state potential energy surface. *Physical Chemistry Chemical Physics*, **2019**, 21, 12667-12675 | 3.6 | 19 |
| 173 | A new full-dimensional ab initio intermolecular potential energy surface and vibrational states for (HF) and (DF). *Journal of Chemical Physics*, **2019**, 150, 154302 | 3.9 | 11 |
| 172 | Hydroxyl super rotors from vacuum ultraviolet photodissociation of water. *Nature Communications*, **2019**, 10, 1250 | 17.4 | 21 |
| 171 | An interaction-asymptotic region decomposition method for general state-to-state reactive scatterings. *Journal of Chemical Physics*, **2019**, 150, 134105 | 3.9 | 14 |
| 170 | Nonadiabatic Dynamics in Photodissociation of Hydroxymethyl in the 3A(3p ) Rydberg State: A Nine-Dimensional Quantum Study. *Journal of Physical Chemistry A*, **2019**, 123, 1937-1944 | 2.8 | 7 |
| 169 | A novel phosphotungstic acid-supported single metal atom catalyst with high activity and selectivity for the synthesis of NH3 from electrochemical N2 reduction: a DFT prediction. *Journal of Materials Chemistry A*, **2019**, 7, 19838-19845 | 13 | 40 |
| 168 | Breakdown of energy transfer gap laws revealed by full-dimensional quantum scattering between HF molecules. *Nature Communications*, **2019**, 10, 4658 | 17.4 | 7 |
| 167 | Identification of the Band Gap Energy of Two-dimensional (OA)(MA)PbI Perovskite with up to 10 Layers. *Journal of Physical Chemistry Letters*, **2019**, 10, 7025-7030 | 6.4 | 11 |
| 166 | Dynamical interference in the vibronic bond breaking reaction of HCO. *Science Advances*, **2019**, 5, eaau0582 | 13.3 | 7 |
| 165 | Quantum dynamics of vibration-vibration energy transfer for vibrationally excited HF colliding with H. *Journal of Computational Chemistry*, **2019**, 40, 1084-1090 | 3.5 | 7 |
| 164 | Quantum dynamics of ClHO photodetachment: Isotope effect and impact of anion vibrational excitation. *Journal of Chemical Physics*, **2018**, 148, 064305 | 3.9 | 4 |

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| 163 | A full-dimensional ab initio potential energy surface and rovibrational energies of the Ar–HF complex. *Molecular Physics*, **2018**, 116, 835-842 | 1.7 | 6 |
| 162 | Signatures of a Conical Intersection in Adiabatic Dissociation on the Ground Electronic State. *Journal of the American Chemical Society*, **2018**, 140, 1986-1989 | 16.4 | 31 |
| 161 | An improved coupled-states approximation including the nearest neighbor Coriolis couplings for diatom-diatom inelastic collision. *Journal of Chemical Physics*, **2018**, 148, 084101 | 3.9 | 12 |
| 160 | Nature of Photoinduced Quenching Traps in Methylammonium Lead Triiodide Perovskite Revealed by Reversible Photoluminescence Decline. *ACS Photonics*, **2018**, 5, 2034-2043 | 6.3 | 36 |
| 159 | Precisely Controlled Incorporation of Drug Nanoparticles in Polymer Vesicles by Amphiphilic Copolymer Tethers. *Macromolecules*, **2018**, 51, 6810-6817 | 5.5 | 9 |
| 158 | Single atom detachment from Cu clusters, and diffusion and trapping on CeO(111): implications in Ostwald ripening and atomic redispersion. *Nanoscale*, **2018**, 10, 17893-17901 | 7.7 | 25 |
| 157 | Vibrational enhancement in the dynamics of ammonia dissociative chemisorption on Ru(0001). *Journal of Chemical Physics*, **2018**, 149, 044703 | 3.9 | 14 |
| 156 | State-to-state photodissociation dynamics of the water molecule. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1350 | 7.9 | 20 |
| 155 | Cover Image, Volume 8, Issue 2. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1362 | 7.9 | 1 |
| 154 | Predicted infrared spectra in the HF stretching band of the H-HF complex. *Journal of Chemical Physics*, **2018**, 149, 094307 | 3.9 | 6 |
| 153 | Modified Gaussian Wave Packet Method for Calculating Initial State Wave Functions in Photodissociation. *Journal of Chemical Theory and Computation*, **2018**, 14, 5527-5534 | 6.4 | 2 |
| 152 | Quantum wavepacket method for state-to-state reactive cross sections in hyperspherical coordinates. *Journal of Chemical Physics*, **2018**, 149, 174103 | 3.9 | 11 |
| 151 | Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in Solution. *Journal of Chemical Theory and Computation*, **2018**, 14, 5787-5796 | 6.4 | 13 |
| 150 | Nonadiabatic Effect in Photodissociation Dynamics of Thiophenol via the $^1\pi\sigma^*$ State. *Journal of Physical Chemistry A*, **2018**, 122, 5375-5382 | 2.8 | 6 |
| 149 | A full-dimensional potential energy surface and quantum dynamics of inelastic collision process for H-HF. *Journal of Chemical Physics*, **2018**, 148, 184301 | 3.9 | 13 |
| 148 | Dynamics of carbon monoxide dissociation on Co(112[combining macron]0). *Physical Chemistry Chemical Physics*, **2017**, 19, 12826-12837 | 3.6 | 8 |
| 147 | A global coupled cluster potential energy surface for HCl + OH <-> Cl + HO. *Physical Chemistry Chemical Physics*, **2017**, 19, 9770-9777 | 3.6 | 13 |
| 146 | Three-Dimensional Diabatic Potential Energy Surfaces for the Photodissociation of Thiophenol. *Journal of Physical Chemistry A*, **2017**, 121, 8432-8439 | 2.8 | 11 |

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| 145 | Nanoparticle encapsulation in vesicles formed by amphiphilic diblock copolymers. *Soft Matter*, **2017**, 13, 7840-7847 | 3.6 | 17 |
| 144 | Accurate Determination of Tunneling-Affected Rate Coefficients: Theory Assessing Experiment. *Journal of Physical Chemistry Letters*, **2017**, 8, 3392-3397 | 6.4 | 19 |
| 143 | Quantum dynamics of polyatomic dissociative chemisorption on transition metal surfaces: mode specificity and bond selectivity. *Chemical Society Reviews*, **2016**, 45, 3621-40 | 58.5 | 117 |
| 142 | Nonadiabatic Tunneling in Photodissociation of Phenol. *Journal of the American Chemical Society*, **2016**, 138, 7828-31 | 16.4 | 102 |
| 141 | Amide Rotation Hindrance Predicts Proteolytic Resistance of Cystine-Knot Peptides. *Journal of Physical Chemistry Letters*, **2016**, 7, 1138-42 | 6.4 | 5 |
| 140 | Rate Coefficients of the HCl + OH -> Cl + H2O Reaction from Ring Polymer Molecular Dynamics. *Journal of Physical Chemistry A*, **2016**, 120, 3433-40 | 2.8 | 30 |
| 139 | Full-Dimensional Quantum Dynamics of Vibrational Mediated Photodissociation of HOD in Its B Band. *Journal of Physical Chemistry A*, **2015**, 119, 12062-72 | 2.8 | 8 |
| 138 | State-to-state reaction dynamics for the reactions of atom N with radicals. *International Journal of Quantum Chemistry*, **2015**, 115, 596-606 | 2.1 | 0 |
| 137 | Six-dimensional quantum dynamics of dissociative chemisorption of H2 on Co(0001) on an accurate global potential energy surface. *Physical Chemistry Chemical Physics*, **2015**, 17, 23346-55 | 3.6 | 20 |
| 136 | A permutationally invariant full-dimensional ab initio potential energy surface for the abstraction and exchange channels of the H + CH4 system. *Journal of Chemical Physics*, **2015**, 142, 204302 | 3.9 | 59 |
| 135 | Mechanistic insights into a classic wonder drug--aspirin. *Journal of the American Chemical Society*, **2015**, 137, 70-3 | 16.4 | 50 |
| 134 | Site-specific dissociation dynamics of H2/D2 on Ag(111) and Co(0001) and the validity of the site-averaging model. *Journal of Chemical Physics*, **2015**, 143, 114706 | 3.9 | 30 |
| 133 | Communication: On the competition between adiabatic and nonadiabatic dynamics in vibrationally mediated ammonia photodissociation in its A band. *Journal of Chemical Physics*, **2015**, 142, 091101 | 3.9 | 26 |
| 132 | Signatures of non-adiabatic dynamics in the fine-structure state distributions of the OH(X /□) products in the B-band photodissociation of H2O. *Journal of Chemical Physics*, **2015**, 142, 124317 | 3.9 | 19 |
| 131 | Theoretical study of the state-to-state photodissociation dynamics of the vibrationally excited water molecule in the B band. *Journal of Physical Chemistry A*, **2014**, 118, 9220-7 | 2.8 | 8 |
| 130 | An experimental and theoretical investigation of the N(S) + C(□g+) reaction at low temperature. *Physical Chemistry Chemical Physics*, **2014**, 16, 14212-9 | 3.6 | 15 |
| 129 | Full-Dimensional Quantum State-to-State Nonadiabatic Dynamics for Photodissociation of Ammonia in its A-Band. *Journal of Physical Chemistry Letters*, **2014**, 5, 1055-60 | 6.4 | 44 |
| 128 | Communication: Rigorous quantum dynamics of O + O2 exchange reactions on an ab initio potential energy surface substantiate the negative temperature dependence of rate coefficients. *Journal of Chemical Physics*, **2014**, 141, 081102 | 3.9 | 30 |

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| 127 | High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate (CH2OO). *Journal of Physical Chemistry Letters*, **2014**, 5, 2364-9 | 6.4 | 79 |
| 126 | State-to-state quantum dynamics of the N(4S) + C2((tilde{X}) 1Σ) -> CN((tilde{X}) 2Σ) + C(3P) reaction. *Theoretical Chemistry Accounts*, **2014**, 133, 1 | 1.9 | 2 |
| 125 | Dissociative chemisorption dynamics of small molecules on metal surfaces. *Science China Chemistry*, **2014**, 57, 87-99 | 7.9 | 1 |
| 124 | Full-dimensional quantum dynamics of vibrationally mediated photodissociation of NH3 and ND3 on coupled ab initio potential energy surfaces: absorption spectra and NH2(Ã(2)A1)/NH2(X (2)B1) branching ratios. *Journal of Physical Chemistry A*, **2014**, 118, 11926-34 | 2.8 | 25 |
| 123 | A tribute to Guosen Yan. *Theoretical Chemistry Accounts*, **2014**, 133, 1 | 1.9 | |
| 122 | Product fine-structure resolved photodissociation dynamics: the A band of H2O. *Journal of Chemical Physics*, **2014**, 140, 024310 | 3.9 | 19 |
| 121 | Low temperature rate constants for the N(4S) + CH(X2Π) reaction. Implications for N2 formation cycles in dense interstellar clouds. *Physical Chemistry Chemical Physics*, **2013**, 15, 13888-96 | 3.6 | 28 |
| 120 | Interaction specific binding hotspots in Endonuclease colicin-immunity protein complex from MD simulations. *Science China Chemistry*, **2013**, 56, 1143-1151 | 7.9 | 6 |
| 119 | Ab initio determination of potential energy surfaces for the first two UV absorption bands of SO2. *Journal of Chemical Physics*, **2013**, 139, 014305 | 3.9 | 34 |
| 118 | Vibrationally mediated bond selective dissociative chemisorption of HOD on Cu(111). *Chemical Science*, **2013**, 4, 503-508 | 9.4 | 54 |
| 117 | Mode selectivity in methane dissociative chemisorption on Ni(111). *Chemical Science*, **2013**, 4, 3249 | 9.4 | 111 |
| 116 | Biomimetic membrane control of block copolymer vesicles with tunable wall thickness. *Soft Matter*, **2013**, 9, 2434 | 3.6 | 24 |
| 115 | State-to-state photodissociation dynamics of H2O in the B-band: competition between two coexisting nonadiabatic pathways. *Journal of Physical Chemistry A*, **2013**, 117, 6940-7 | 2.8 | 33 |
| 114 | Influence of Step Defects on Methanol Decomposition: Periodic Density Functional Studies on Pd(211) and Kinetic Monte Carlo Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 451-459 | 3.8 | 26 |
| 113 | Effects of reactant internal excitation and orientation on dissociative chemisorption of H2O on Cu(111): quasi-seven-dimensional quantum dynamics on a refined potential energy surface. *Journal of Chemical Physics*, **2013**, 138, 044704 | 3.9 | 54 |
| 112 | Vibronic origin of sulfur mass-independent isotope effect in photoexcitation of SO2 and the implications to the early earth's atmosphere. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 17697-702 | 11.5 | 77 |
| 111 | State-to-state quantum dynamics of the O(3P) + NH(X3Σ-)) reaction on the three lowest-lying electronic states of HNO/HON. *Journal of Chemical Physics*, **2013**, 138, 024308 | 3.9 | 6 |
| 110 | A new six-dimensional potential energy surface for H2-N2O and its adiabatic-hindered-rotor treatment. *Journal of Chemical Physics*, **2013**, 139, 034312 | 3.9 | 24 |

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| 109 | State-to-state quantum dynamics of the N(4S) + CH(X2Π) -> CN(X2Σ+,A2Π) + H(2S) reactions. *Journal of Chemical Physics*, **2013**, 139, 124313 | 3.9 | 5 |
| 108 | State to state photodissociation dynamics of D2O in the B band. *Journal of Chemical Physics*, **2013**, 139, 114303 | 3.9 | 11 |
| 107 | First-principles study of the methyl formate pathway of methanol steam reforming on PdZn(1 1 1) with comparison to Cu(1 1 1). *Journal of Molecular Catalysis A*, **2012**, 356, 165-170 | | 24 |
| 106 | Initial Decomposition of Methanol and Water on In2O3(110): A Periodic DFT Study. *Chinese Journal of Chemistry*, **2012**, 30, 2036-2040 | 4.9 | 11 |
| 105 | Communication: a chemically accurate global potential energy surface for the HO + CO -> H + CO2 reaction. *Journal of Chemical Physics*, **2012**, 136, 041103 | 3.9 | 95 |
| 104 | Controlling the self-assembly pathways of amphiphilic block copolymers into vesicles. *Soft Matter*, **2012**, 8, 7865 | 3.6 | 48 |
| 103 | Ab Initio Potential Energy Surfaces for Both the Ground (X 1A?) and Excited (A~1A??) Electronic States of HSiBr and the Absorption and Emission Spectra of HSiBr/DSiBr. *Advances in Physical Chemistry*, **2012**, 2012, 1-20 | | 28 |
| 102 | State-to-state photodissociation dynamics of triatomic molecules: H2O in the B band. *Journal of Chemical Physics*, **2012**, 136, 034302 | 3.9 | 46 |
| 101 | A new four-dimensional ab initio potential energy surface for N2O-He and vibrational band origin shifts for the N2O-He(N) clusters with N = 1-40. *Journal of Chemical Physics*, **2012**, 137, 104311 | 3.9 | 28 |
| 100 | Enhancing dissociative chemisorption of H2O on Cu(111) via vibrational excitation. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 10224-7 | 11.5 | 82 |
| 99 | Pathways for methanol steam reforming involving adsorbed formaldehyde and hydroxyl intermediates on Cu(111): density functional theory studies. *Physical Chemistry Chemical Physics*, **2011**, 13, 9622-31 | 3.6 | 48 |
| 98 | Methyl Formate Pathway in Methanol Steam Reforming on Copper: Density Functional Calculations. *ACS Catalysis*, **2011**, 1, 1263-1271 | 13.1 | 38 |
| 97 | New ab initio coupled potential energy surfaces for the Br(2P(3/2), 2P(1/2)) + H2 reaction. *Journal of Chemical Physics*, **2011**, 135, 164311 | 3.9 | 10 |
| 96 | Communication: state-to-state differential cross sections for H2O(B ) photodissociation. *Journal of Chemical Physics*, **2011**, 134, 231103 | 3.9 | 19 |
| 95 | Intermolecular potential energy surface, microwave and infrared spectra of the Kr–CO2 complex from ab initio calculations. *Chemical Physics Letters*, **2011**, 511, 229-234 | 2.5 | 23 |
| 94 | New ab initio potential energy surfaces for both the ground (X 1A′) and excited (1A?) electronic states of HSiCl and the absorption and emission spectra of HSiCl/DSiCl. *Journal of Computational Chemistry*, **2011**, 32, 1694-702 | 3.5 | 2 |
| 93 | Pathways of Methanol Steam Reforming on PdZn and Comparison with Cu. *Journal of Physical Chemistry C*, **2011**, 115, 20583-20589 | 3.8 | 51 |
| 92 | Superfluid response of 4HeN–N2O clusters probed by path integral Monte Carlo simulations. *Journal of Molecular Spectroscopy*, **2011**, 267, 136-143 | 1.3 | 14 |

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| 91 | Initial steps in methanol steam reforming on PdZn and ZnO surfaces: Density functional theory studies. *Surface Science*, **2011**, 605, 750-759 | 1.8 | 46 |
| 90 | A new ab initio potential energy surface and microwave and infrared spectra for the Ne-CO(2) complex. *Journal of Chemical Physics*, **2010**, 133, 104302 | 3.9 | 27 |
| 89 | State-to-state quantum dynamics of the O(3P)+OH(2Pi)-->H(2S)+O2(3Sigma(g)-) reaction. *Journal of Chemical Physics*, **2010**, 133, 054302 | 3.9 | 31 |
| 88 | Nonadiabatic dynamics of A-state photodissociation of ammonia: a four-dimensional wave packet study. *Journal of Physical Chemistry A*, **2010**, 114, 3121-6 | 2.8 | 16 |
| 87 | A new potential energy surface and predicted infrared spectra of the Ar-CO(2) van der Waals complex. *Journal of Chemical Physics*, **2009**, 130, 224311 | 3.9 | 38 |
| 86 | N(2)O in small para-hydrogen clusters: Structures and energetics. *Journal of Computational Chemistry*, **2009**, 30, 841-6 | 3.5 | 5 |
| 85 | Theoretical prediction of the noble gas complexes HeAuF and NeAuF. *Science in China Series B: Chemistry*, **2009**, 52, 1987-1990 | | 9 |
| 84 | Effects of reactant rotational excitation on H + O2--> OH + O reaction rate constant: quantum wave packet, quasi-classical trajectory and phase space theory calculations. *Physical Chemistry Chemical Physics*, **2009**, 11, 4715-21 | 3.6 | 15 |
| 83 | Ab initio potential energy surfaces for the ground (X1A′) and excited (A1A″) electronic states of HGeBr and the Absorption and emission spectra of HGeBr/DGeBr. *Journal of Physical Chemistry A*, **2009**, 113, 7314-21 | 2.8 | 3 |
| 82 | Fully Coriolis-coupled quantum studies of the H + O2 (upsilon i = 0-2, j i = 0,1) --> OH + O reaction on an accurate potential energy surface: integral cross sections and rate constants. *Journal of Physical Chemistry A*, **2008**, 112, 602-11 | 2.8 | 44 |
| 81 | State-to-state dynamics of H + O2 reaction, evidence for nonstatistical behavior. *Journal of the American Chemical Society*, **2008**, 130, 14962-3 | 16.4 | 46 |
| 80 | A new potential energy surface and predicted infrared spectra of He-CO2: dependence on the antisymmetric stretch of CO2. *Journal of Chemical Physics*, **2008**, 128, 124323 | 3.9 | 40 |
| 79 | VIBRATIONALLY AVERAGED POTENTIAL ENERGY SURFACES AND PREDICTED INFRARED SPECTRA OF THE He–18O13C18O AND He–16O13C16O COMPLEXES. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 707-717 | 1.8 | 7 |
| 78 | Full-dimensional quantum dynamics of A-state photodissociation of ammonia: absorption spectra. *Journal of Chemical Physics*, **2008**, 129, 154311 | 3.9 | 25 |
| 77 | Accurate quantum mechanical calculations of differential and integral cross sections and rate constant for the O+OH reaction using an ab initio potential energy surface. *Journal of Chemical Physics*, **2008**, 128, 014303 | 3.9 | 56 |
| 76 | Path integral Monte Carlo study of CO2 solvation in 4He clusters. *Journal of Chemical Physics*, **2008**, 128, 224513 | 3.9 | 17 |
| 75 | Ab initio potential energy surfaces for both the ground (X (1)A′) and excited (A (1)A") electronic states of HGeCl and the absorption and emission spectra of HGeCl/DGeCl. *Journal of Chemical Physics*, **2008**, 129, 154313 | 3.9 | 5 |
| 74 | Theoretical study of adsorption and dissociation of NH3 on the Ir{110}(1×2) surface. *Science Bulletin* , **2008**, 53, 3169-3172 | 10.6 | 4 |

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|---|---|---|---|
| 73 | Mechanistic insights into the H+O2->OH+O reaction from quasi-classical trajectory studies on a new ab initio potential energy surface. *Chemical Physics*, **2008**, 349, 181-187 | 2.3 | 17 |
| 72 | First-principles study of decomposition of NH3 on Ir(100). *Surface Science*, **2008**, 602, 1288-1294 | 1.8 | 46 |
| 71 | Supermolecule density functional calculations suggest a key role for solvent in alkaline hydrolysis of p-nitrophenyl phosphate. *Chemical Communications*, **2007**, 1638-40 | 5.8 | 40 |
| 70 | Electronic excitations of green fluorescent proteins: modeling solvatochromatic shifts of red fluorescent protein chromophore model compound in aqueous solutions. *Journal of Physical Chemistry B*, **2007**, 111, 14055-63 | 3.4 | 19 |
| 69 | Differential and integral cross sections for the H + O2 --> OH + O combustion reaction. *Journal of Physical Chemistry A*, **2007**, 111, 5349-52 | 2.8 | 42 |
| 68 | Theoretical investigation on the GaCl3-catalyzed ring-closing metathesis reaction of N-2,3-butadienyl-2-propynyl-1-amine: three-membered ring versus four-membered ring mechanism. *Journal of Physical Chemistry A*, **2007**, 111, 9387-92 | 2.8 | 7 |
| 67 | Global analytical potential energy surfaces for HO2(X2A") based on high-level ab initio calculations. *Journal of Chemical Physics*, **2007**, 126, 074315 | 3.9 | 43 |
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