

# Daiqian Xie

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Observation of Feshbach resonances in the $F + H_2 \rightarrow HF + H$ reaction. <i>Science</i> , <b>2006</b> , 311, 1440-3	33.3	260
215	Quantum dynamics of polyatomic dissociative chemisorption on transition metal surfaces: mode specificity and bond selectivity. <i>Chemical Society Reviews</i> , <b>2016</b> , 45, 3621-40	58.5	117
214	Mode selectivity in methane dissociative chemisorption on Ni(111). <i>Chemical Science</i> , <b>2013</b> , 4, 3249	9.4	111
213	Nonadiabatic Tunneling in Photodissociation of Phenol. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 7828-31	16.4	102
212	A new ab initio potential-energy surface of $HO_2(X^2A'')$ and quantum studies of $HO_2$ vibrational spectrum and rate constants for the $H + O_2 \rightarrow O + OH$ reactions. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 244305	3.9	101
211	Communication: a chemically accurate global potential energy surface for the $HO + CO \rightarrow H + CO_2$ reaction. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 041103	3.9	95
210	Enhancing dissociative chemisorption of $H_2O$ on Cu(111) via vibrational excitation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2012</b> , 109, 10224-7	11.5	82
209	High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate ( $CH_2OO$ ). <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 2364-9	6.4	79
208	Vibronic origin of sulfur mass-independent isotope effect in photoexcitation of $SO_2$ and the implications to the early earth atmosphere. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2013</b> , 110, 17697-702	11.5	77
207	A permutationally invariant full-dimensional ab initio potential energy surface for the abstraction and exchange channels of the $H + CH_4$ system. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 204302	3.9	59
206	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. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 014303	3.9	56
205	Three-Dimensional Photodissociation Dynamics of Rotational State Selected Methyl Iodide. <i>Journal of Physical Chemistry A</i> , <b>2000</b> , 104, 1009-1019	2.8	55
204	Vibrationally mediated bond selective dissociative chemisorption of $HOD$ on Cu(111). <i>Chemical Science</i> , <b>2013</b> , 4, 503-508	9.4	54
203	Effects of reactant internal excitation and orientation on dissociative chemisorption of $H_2O$ on Cu(111): quasi-seven-dimensional quantum dynamics on a refined potential energy surface. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 044704	3.9	54
202	Rate constant for $OH(2 \Pi) + O(3P) \rightarrow H(2S) + O_2(3 \Sigma g^-)$ reaction on an improved ab initio potential energy surface and implications for the interstellar oxygen problem. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 024304	3.9	52
201	Pathways of Methanol Steam Reforming on PdZn and Comparison with Cu. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 20583-20589	3.8	51
200	Ab initio potential energy surface and rovibrational spectra of $He-O_2$ . <i>Journal of Chemical Physics</i> , <b>1998</b> , 109, 10284-10292	3.9	51

199	Mechanistic insights into a classic wonder drug--aspirin. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 70-3	16.4	50
198	Controlling the self-assembly pathways of amphiphilic block copolymers into vesicles. <i>Soft Matter</i> , <b>2012</b> , 8, 7865	3.6	48
197	Pathways for methanol steam reforming involving adsorbed formaldehyde and hydroxyl intermediates on Cu(111): density functional theory studies. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 9622-31	3.6	48
196	Initial steps in methanol steam reforming on PdZn and ZnO surfaces: Density functional theory studies. <i>Surface Science</i> , <b>2011</b> , 605, 750-759	1.8	46
195	State-to-state photodissociation dynamics of triatomic molecules: H <sub>2</sub> O in the B band. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 034302	3.9	46
194	State-to-state dynamics of H + O <sub>2</sub> reaction, evidence for nonstatistical behavior. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 14962-3	16.4	46
193	First-principles study of decomposition of NH <sub>3</sub> on Ir(100). <i>Surface Science</i> , <b>2008</b> , 602, 1288-1294	1.8	46
192	Full-Dimensional Quantum State-to-State Nonadiabatic Dynamics for Photodissociation of Ammonia in its A-Band. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 1055-60	6.4	44
191	Fully Coriolis-coupled quantum studies of the H + O <sub>2</sub> (upsilon i = 0-2, j i = 0,1) --> OH + O reaction on an accurate potential energy surface: integral cross sections and rate constants. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 602-11	2.8	44
190	Global analytical potential energy surfaces for HO <sub>2</sub> (X <sup>2</sup> A'') based on high-level ab initio calculations. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 074315	3.9	43
189	Cobalt/zinc dual-sites coordinated with nitrogen in nanofibers enabling efficient and durable oxygen reduction reaction in acidic fuel cells. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 3686-3691	13	42
188	Differential and integral cross sections for the H + O <sub>2</sub> --> OH + O combustion reaction. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 5349-52	2.8	42
187	A novel phosphotungstic acid-supported single metal atom catalyst with high activity and selectivity for the synthesis of NH <sub>3</sub> from electrochemical N <sub>2</sub> reduction: a DFT prediction. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 19838-19845	13	40
186	A new potential energy surface and predicted infrared spectra of He-CO <sub>2</sub> : dependence on the antisymmetric stretch of CO <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 124323	3.9	40
185	Supermolecule density functional calculations suggest a key role for solvent in alkaline hydrolysis of p-nitrophenyl phosphate. <i>Chemical Communications</i> , <b>2007</b> , 1638-40	5.8	40
184	Quantum dynamics of the H + O <sub>2</sub> --> O + OH reaction on an accurate ab initio potential energy surface. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 23641-3	3.4	40
183	Density functional theory studies on molecular structure and IR spectra of 9-methyladenine: A scaled quantum mechanical force field approach. <i>International Journal of Quantum Chemistry</i> , <b>2000</b> , 76, 686-699	2.1	40
182	Methyl Formate Pathway in Methanol Steam Reforming on Copper: Density Functional Calculations. <i>ACS Catalysis</i> , <b>2011</b> , 1, 1263-1271	13.1	38

181	A new potential energy surface and predicted infrared spectra of the Ar-CO(2) van der Waals complex. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 224311	3.9	38
180	Analysis of the HO2 vibrational spectrum on an accurate ab initio potential energy surface. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 10353-61	2.8	37
179	Comparison of Chebyshev, Faber, and Lanczos propagation-based methods for calculating resonances. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 5263-5269	3.9	37
178	Nature of Photoinduced Quenching Traps in Methylammonium Lead Triiodide Perovskite Revealed by Reversible Photoluminescence Decline. <i>ACS Photonics</i> , <b>2018</b> , 5, 2034-2043	6.3	36
177	Theoretical studies of . <i>Chemical Physics Letters</i> , <b>2007</b> , 439, 280-283	2.5	36
176	Five-dimensional ab initio potential energy surface and predicted infrared spectra of H2-CO2 van der Waals complexes. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 204304	3.9	36
175	Potential energy surfaces and predicted infrared spectra for van der Waals complexes: dependence on one intramolecular vibrational coordinate. <i>International Reviews in Physical Chemistry</i> , <b>2007</b> , 26, 487-520	7.0	35
174	CALCULATION OF TRANSITION AMPLITUDES WITH A SINGLE LANCZOS PROPAGATION. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2002</b> , 01, 173-185	1.8	35
173	Ab initio determination of potential energy surfaces for the first two UV absorption bands of SO2. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 014305	3.9	34
172	State-to-state photodissociation dynamics of H2O in the B-band: competition between two coexisting nonadiabatic pathways. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 6940-7	2.8	33
171	Electronic excitations of green fluorescent proteins: protonation states of chromophore model compound in solutions. <i>Journal of Computational Chemistry</i> , <b>2005</b> , 26, 1487-96	3.5	32
170	Signatures of a Conical Intersection in Adiabatic Dissociation on the Ground Electronic State. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 1986-1989	16.4	31
169	State-to-state quantum dynamics of the O(3P)+OH(2Pi)-->H(2S)+O2(3Sigma(g)-) reaction. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 054302	3.9	31
168	Communication: Rigorous quantum dynamics of O + O2 exchange reactions on an ab initio potential energy surface substantiate the negative temperature dependence of rate coefficients. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 081102	3.9	30
167	Site-specific dissociation dynamics of H2/D2 on Ag(111) and Co(0001) and the validity of the site-averaging model. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 114706	3.9	30
166	Intermolecular potential energy surface and rovibrational spectra of the He-N2O complex from ab initio calculations. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 8575-81	3.9	30
165	Rate Coefficients of the HCl + OH -> Cl + H2O Reaction from Ring Polymer Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 3433-40	2.8	30
164	Low temperature rate constants for the N(4S) + CH(X2E) reaction. Implications for N2 formation cycles in dense interstellar clouds. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 13888-96	3.6	28

163	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. <i>Advances in Physical Chemistry</i> , <b>2012</b> , 2012, 1-20		28
162	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. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 104311	3.9	28
161	A new ab initio potential energy surface and microwave and infrared spectra for the Ne-CO(2) complex. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 104302	3.9	27
160	Revelation of non-statistical behavior in HO2 vibration by a new ab initio potential energy surface. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 091103	3.9	27
159	Advances and New Challenges to Bimolecular Reaction Dynamics Theory. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 8844-8860	6.4	27
158	Communication: On the competition between adiabatic and nonadiabatic dynamics in vibrationally mediated ammonia photodissociation in its A band. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 091101	3.9	26
157	Influence of Step Defects on Methanol Decomposition: Periodic Density Functional Studies on Pd(211) and Kinetic Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 451-459	3.8	26
156	A three-dimensional ab initio potential energy surface and predicted infrared spectra for the He-N2O complex. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 144317	3.9	26
155	Solvent effect on concertedness of the transition state in the hydrolysis of p-nitrophenyl acetate. <i>Organic Letters</i> , <b>2005</b> , 7, 2093-5	6.2	26
154	A theoretical study of solvent effects on tautomerism and electronic absorption spectra of 3-hydroxy-2-mercaptopyridine and 2,3-dihydroxypyridine. <i>Journal of Computational Chemistry</i> , <b>2004</b> , 25, 1833-9	3.5	26
153	Absorption and resonance emission spectra of SO2(X 1A1/C 1B2) calculated from ab initio potential energy and transition dipole moment surfaces. <i>Chemical Physics Letters</i> , <b>2000</b> , 329, 503-510	2.5	26
152	Single atom detachment from Cu clusters, and diffusion and trapping on CeO(111): implications in Ostwald ripening and atomic redispersion. <i>Nanoscale</i> , <b>2018</b> , 10, 17893-17901	7.7	25
151	Full-dimensional quantum dynamics of vibrationally mediated photodissociation of NH3 and ND3 on coupled ab initio potential energy surfaces: absorption spectra and NH2(2A1)/NH2(X (2)B1) branching ratios. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 11926-34	2.8	25
150	Full-dimensional quantum dynamics of A-state photodissociation of ammonia: absorption spectra. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 154311	3.9	25
149	Mode Specificity in the OH + HO -> HO + O Reaction: Enhancement of Reactivity by Exciting a Spectator Mode. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 3331-3335	16.4	24
148	First-principles study of the methyl formate pathway of methanol steam reforming on PdZn(1 1 1) with comparison to Cu(1 1 1). <i>Journal of Molecular Catalysis A</i> , <b>2012</b> , 356, 165-170		24
147	Biomimetic membrane control of block copolymer vesicles with tunable wall thickness. <i>Soft Matter</i> , <b>2013</b> , 9, 2434	3.6	24
146	A new six-dimensional potential energy surface for H2-N2O and its adiabatic-hindered-rotor treatment. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 034312	3.9	24

145	Theoretical study of predissociation dynamics of HCN/DCN in their first absorption bands. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 10626-10635	3.9	24
144	Intermolecular potential energy surface, microwave and infrared spectra of the KrNO <sub>2</sub> complex from ab initio calculations. <i>Chemical Physics Letters</i> , <b>2011</b> , 511, 229-234	2.5	23
143	Hydroxyl super rotors from vacuum ultraviolet photodissociation of water. <i>Nature Communications</i> , <b>2019</b> , 10, 1250	17.4	21
142	Quantum calculations of highly excited vibrational spectrum of sulfur dioxide. III. Emission spectra from the C 1B <sub>2</sub> state. <i>Journal of Chemical Physics</i> , <b>1999</b> , 111, 7782-7788	3.9	21
141	Precision test of statistical dynamics with state-to-state ultracold chemistry. <i>Nature</i> , <b>2021</b> , 593, 379-384	50.4	21
140	Six-dimensional quantum dynamics of dissociative chemisorption of H <sub>2</sub> on Co(0001) on an accurate global potential energy surface. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 23346-55	3.6	20
139	Hydrogen bonding and solvatochromatic shift of the lowest 1(n, pi*) excitation of s-tetrazine in its hydrated clusters and dilute solutions. <i>Journal of Computational Chemistry</i> , <b>2004</b> , 25, 1487-94	3.5	20
138	An ab initio potential energy surface and predissociative resonances of HArF. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 4273-80	3.9	20
137	State-to-state photodissociation dynamics of the water molecule. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2018</b> , 8, e1350	7.9	20
136	Anomalous kinetics of the reaction between OH and HO on an accurate triplet state potential energy surface. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 12667-12675	3.6	19
135	Accurate Determination of Tunneling-Affected Rate Coefficients: Theory Assessing Experiment. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 3392-3397	6.4	19
134	Signatures of non-adiabatic dynamics in the fine-structure state distributions of the OH(X <sup>2</sup> Π) products in the B-band photodissociation of H <sub>2</sub> O. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 124317	3.9	19
133	Product fine-structure resolved photodissociation dynamics: the A band of H <sub>2</sub> O. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 024310	3.9	19
132	Communication: state-to-state differential cross sections for H <sub>2</sub> O(B <sup>2</sup> Σ <sup>+</sup> ) photodissociation. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 231103	3.9	19
131	Electronic excitations of green fluorescent proteins: modeling solvatochromatic shifts of red fluorescent protein chromophore model compound in aqueous solutions. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 14055-63	3.4	19
130	A five-dimensional potential energy surface and predicted infrared spectra for the N <sub>2</sub> O-hydrogen complexes. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 174310	3.9	19
129	Theoretical studies for structures and energetics of Rgn-N <sub>2</sub> O (Rg=He, Ne, Ar) clusters. <i>Journal of Computational Chemistry</i> , <b>2003</b> , 24, 1839-45	3.5	19
128	Direct calculation of cumulative reaction probabilities from Chebyshev correlation functions. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 6391-6396	3.9	19

127	Nanoparticle encapsulation in vesicles formed by amphiphilic diblock copolymers. <i>Soft Matter</i> , <b>2017</b> , 13, 7840-7847	3.6	17
126	Path integral Monte Carlo study of CO <sub>2</sub> solvation in 4He clusters. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 224513	3.9	17
125	Mechanistic insights into the H+O <sub>2</sub> ->OH+O reaction from quasi-classical trajectory studies on a new ab initio potential energy surface. <i>Chemical Physics</i> , <b>2008</b> , 349, 181-187	2.3	17
124	A refined potential energy function for the electronic ground state of NO <sub>2</sub> . <i>Molecular Physics</i> , <b>1996</b> , 88, 1349-1355	1.7	17
123	Nonadiabatic dynamics of A-state photodissociation of ammonia: a four-dimensional wave packet study. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 3121-6	2.8	16
122	Ab initio potential energy surface and predicted microwave spectra for Ar--OCS dimer and structures of Ar <sub>n</sub> --OCS (n = 2-14) clusters. <i>Journal of Computational Chemistry</i> , <b>2006</b> , 27, 1045-53	3.5	16
121	Density functional study of the adsorption of Na and K on Rh(1 1 1). <i>Surface Science</i> , <b>2004</b> , 553, 13-22	1.8	16
120	Ab initio potential energy surface and rovibrational spectra of NeN <sub>2</sub> O. <i>Chemical Physics Letters</i> , <b>2002</b> , 351, 149-157	2.5	16
119	Medium effects on the lowest 1(n,π*) excitation of 1,2,3-triazine in water. <i>Chemical Physics Letters</i> , <b>2003</b> , 368, 377-383	2.5	16
118	An experimental and theoretical investigation of the N(Σ) + C(CH <sub>3</sub> ) <sub>3</sub> reaction at low temperature. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 14212-9	3.6	15
117	Effects of reactant rotational excitation on H + O <sub>2</sub> --> OH + O reaction rate constant: quantum wave packet, quasi-classical trajectory and phase space theory calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 4715-21	3.6	15
116	Ab initio intermolecular potential-energy surface and microwave spectra for the Ne-OCS complex. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 234312	3.9	15
115	Theoretical Study of the aza-Wittig Reactions of X <sub>3</sub> PNH (X=H and Cl) with Formaldehyde in Gas Phase and in Solution. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 9053-9058	2.8	15
114	Insights into the Mechanism of Nonadiabatic Photodissociation from Product Vibrational Distributions. The Remarkable Case of Phenol. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 191-198	6.4	15
113	An interaction-asymptotic region decomposition method for general state-to-state reactive scatterings. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 134105	3.9	14
112	Vibrational enhancement in the dynamics of ammonia dissociative chemisorption on Ru(0001). <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 044703	3.9	14
111	Superfluid response of 4HeN <sub>2</sub> O clusters probed by path integral Monte Carlo simulations. <i>Journal of Molecular Spectroscopy</i> , <b>2011</b> , 267, 136-143	1.3	14
110	Reactivity of metaphosphate and thiometaphosphate in water: a DFT study. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 11295-303	2.8	14

109	Theoretical studies of force fields and IR spectra of isocytosine. <i>International Journal of Quantum Chemistry</i> , <b>1999</b> , 72, 53-60	2.1	14
108	A global coupled cluster potential energy surface for HCl + OH <-> Cl + HO. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 9770-9777	3.6	13
107	Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in Solution. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 5787-5796	6.4	13
106	A full-dimensional potential energy surface and quantum dynamics of inelastic collision process for H-HF. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 184301	3.9	13
105	A Global Full-Dimensional Potential Energy Surface for the KRb Complex and Its Lifetime. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 2605-2610	6.4	12
104	An improved coupled-states approximation including the nearest neighbor Coriolis couplings for diatom-diatom inelastic collision. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 084101	3.9	12
103	Three-dimensional ab initio potential-energy surface and rovibrational spectra of the H <sub>2</sub> -Kr complex. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 134323	3.9	12
102	Ab initio potential energy surface and rovibrational spectrum of Ar-HCCCN. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 2630-5	3.9	12
101	Theoretical Investigations of Rate Coefficients for H + O and HO + O Reactions on a Full-Dimensional Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 6427-6437	2.8	12
100	Three-Dimensional Diabatic Potential Energy Surfaces for the Photodissociation of Thiophenol. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 8432-8439	2.8	11
99	A new full-dimensional ab initio intermolecular potential energy surface and vibrational states for (HF) and (DF). <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 154302	3.9	11
98	Identification of the Band Gap Energy of Two-dimensional (OA)(MA)PbI Perovskite with up to 10 Layers. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 7025-7030	6.4	11
97	Initial Decomposition of Methanol and Water on In <sub>2</sub> O <sub>3</sub> (110): A Periodic DFT Study. <i>Chinese Journal of Chemistry</i> , <b>2012</b> , 30, 2036-2040	4.9	11
96	State to state photodissociation dynamics of D <sub>2</sub> O in the B band. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 114303	3.9	11
95	Ab initio potential energy surface and excited vibrational states for the electronic ground state of Li <sub>2</sub> H. <i>Science in China Series B: Chemistry</i> , <b>1997</b> , 40, 342-347		11
94	Rovibrational bound states of the NeDCS complex. <i>Chemical Physics Letters</i> , <b>1998</b> , 287, 162-168	2.5	11
93	Theoretical study of general base-catalyzed hydrolysis of aryl esters and implications for enzymatic reactions. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 5259-66	3.4	11
92	A DFT investigation of potential energy surface and vibrational properties of hydrogen adsorbed on the Rh(111) surface. <i>Surface Science</i> , <b>2004</b> , 550, 15-20	1.8	11

91	Quantum wavepacket method for state-to-state reactive cross sections in hyperspherical coordinates. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 174103	3.9	11
90	Statistical quantum mechanical approach to diatom-diatom capture dynamics and application to ultracold KRb + KRb reaction. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 241103	3.9	10
89	New ab initio coupled potential energy surfaces for the Br(2P(3/2), 2P(1/2)) + H2 reaction. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 164311	3.9	10
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87	Precisely Controlled Incorporation of Drug Nanoparticles in Polymer Vesicles by Amphiphilic Copolymer Tethers. <i>Macromolecules</i> , <b>2018</b> , 51, 6810-6817	5.5	9
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