## **Xueming Yang**

List of Publications by Year in descending order

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272 papers 8,774 citations

57758 44 h-index 83 g-index

282 all docs  $\begin{array}{c} 282 \\ \text{docs citations} \end{array}$ 

times ranked

282

6691 citing authors

#	Article	IF	CITATIONS
1	Fundamentals of TiO <sub>2</sub> Photocatalysis: Concepts, Mechanisms, and Challenges. Advanced Materials, 2019, 31, e1901997.	21.0	999
2	Elementary photocatalytic chemistry on TiO <sub>2</sub> surfaces. Chemical Society Reviews, 2016, 45, 3701-3730.	38.1	288
3	Observation of Feshbach Resonances in the F + H2 -> HF + H Reaction. Science, 2006, 311, 1440-1443.	12.6	278
4	Stepwise Photocatalytic Dissociation of Methanol and Water on TiO <sub>2</sub> (110). Journal of the American Chemical Society, 2012, 134, 13366-13373.	13.7	244
5	Single Molecule Photocatalysis on TiO <sub>2</sub> Surfaces. Chemical Reviews, 2019, 119, 11020-11041.	47.7	212
6	Unraveling Charge State of Supported Au Single-Atoms during CO Oxidation. Journal of the American Chemical Society, 2018, 140, 554-557.	13.7	192
7	Photodissociation of H2O at 121.6 nm: A state-to-state dynamical picture. Journal of Chemical Physics, 2000, 113, 10073-10090.	3.0	175
8	Forward scattering due to slow-down of the intermediate in the H + HD â†' D + H2 reaction. Nature, 2002, 419, 281-284.	27.8	169
9	Localized Excitation of Ti <sup>3+</sup> lons in the Photoabsorption and Photocatalytic Activity of Reduced Rutile TiO <sub>2</sub> . Journal of the American Chemical Society, 2015, 137, 9146-9152.	13.7	168
10	Experimental and Theoretical Differential Cross Sections for a Four-Atom Reaction: HD + OH â†' H <sub>2</sub> O + D. Science, 2011, 333, 440-442.	12.6	152
11	Site-specific photocatalytic splitting of methanol on TiO2(110). Chemical Science, 2010, 1, 575.	7.4	150
12	Breakdown of the Born-Oppenheimer Approximation in the F+ <i>o</i> -D <sub>2</sub> â†' DF + D Reaction. Science, 2007, 317, 1061-1064.	12.6	149
13	Self-Assembled Framework Enhances Electronic Communication of Ultrasmall-Sized Nanoparticles for Exceptional Solar Hydrogen Evolution. Journal of the American Chemical Society, 2017, 139, 4789-4796.	13.7	146
14	Interference of Quantized Transition-State Pathways in the H + D2 -> D + HD Chemical Reaction. Science, 2003, 300, 1730-1734.	12.6	137
15	Transition-State Spectroscopy of Partial Wave Resonances in the F + HD Reaction. Science, 2010, 327, $1501-1502$ .	12.6	124
16	Dynamical Resonances Accessible Only by Reagent Vibrational Excitation in the F + HD→HF + D Reaction. Science, 2013, 342, 1499-1502.	12.6	107
17	Molecular Hydrogen Formation from Photocatalysis of Methanol on TiO $<$ sub $>2<$ /sub $>(110)$ . Journal of the American Chemical Society, 2013, 135, 10206-10209.	13.7	102
18	Methyl Formate Production on TiO <sub>2</sub> (110), Initiated by Methanol Photocatalysis at 400 nm. Journal of Physical Chemistry C, 2013, 117, 5293-5300.	3.1	100

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19	Observation of the geometric phase effect in the H + HD → H <sub>2</sub> + D reaction. Science, 2018, 362, 1289-1293.	12.6	99
20	The Extent of Non–Born-Oppenheimer Coupling in the Reaction of Cl( <sup>2</sup> <i>P</i> ) with <i>para-</i> H <sub>2</sub> . Science, 2008, 322, 573-576.	12.6	95
21	State-to-State Dynamics of Elementary Bimolecular Reactions. Annual Review of Physical Chemistry, 2007, 58, 433-459.	10.8	94
22	Metallic Co <sub>2</sub> C: A Promising Co-catalyst To Boost Photocatalytic Hydrogen Evolution of Colloidal Quantum Dots. ACS Catalysis, 2018, 8, 5890-5895.	11.2	92
23	Extremely short-lived reaction resonances in Cl + HD ( $\langle i \rangle v \langle i \rangle = 1$ ) $\hat{a}^{\dagger}$ DCl + H due to chemical bond softening. Science, 2015, 347, 60-63.	12.6	91
24	Molecular Hydrogen Formation from Photocatalysis of Methanol on Anatase-TiO <sub>2</sub> (101). Journal of the American Chemical Society, 2014, 136, 602-605.	13.7	89
25	Photochemistry of the Water Molecule: Adiabatic versus Nonadiabatic Dynamics. Accounts of Chemical Research, 2011, 44, 369-378.	15.6	78
26	Band-Gap States of TiO <sub>2</sub> (110): Major Contribution from Surface Defects. Journal of Physical Chemistry Letters, 2013, 4, 3839-3844.	4.6	76
27	Probing the resonance potential in the F atom reaction with hydrogen deuteride with spectroscopic accuracy. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12662-12666.	7.1	75
28	First-principles quantum dynamical theory for the dissociative chemisorption of H2O on rigid Cu(111). Nature Communications, $2016, 7, 11953$ .	12.8	74
29	HF( $\langle i \rangle v \hat{a} \in 2 \langle  i \rangle = 3$ ) forward scattering in the F + H $\langle sub \rangle 2 \langle  sub \rangle$ reaction: Shape resonance and slow-down mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6227-6231.	7.1	72
30	Nonadiabatic dissociation dynamics in H <sub>2</sub> O: Competition between rotationally and nonrotationally mediated pathways. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 19148-19153.	7.1	68
31	A seven-dimensional quantum dynamics study of the dissociative chemisorption of H <sub>2</sub> O on Cu(111): effects of azimuthal angles and azimuthal angle-averaging. Chemical Science, 2016, 7, 1840-1845.	7.4	64
32	Effect of defects on photocatalytic dissociation of methanol on TiO2(110). Chemical Science, 2011, 2, $1980$ .	7.4	61
33	A fully state- and angle-resolved study of the H+HDâ†'D+H2 reaction: Comparison of a molecular beam experiment to ab initio quantum reaction dynamics. Journal of Chemical Physics, 2002, 117, 8341-8361.	3.0	60
34	Strong Photon Energy Dependence of the Photocatalytic Dissociation Rate of Methanol on TiO <sub>2</sub> (110). Journal of the American Chemical Society, 2013, 135, 19039-19045.	13.7	58
35	In situ formation of mononuclear complexes by reaction-induced atomic dispersion of supported noble metal nanoparticles. Nature Communications, 2019, 10, 5281.	12.8	57
36	Photodissociation of D2O at 121.6 nm: A state-to-state dynamical picture. Journal of Chemical Physics, 2001, 114, 7830-7837.	3.0	55

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37	Infrared spectroscopy of neutral water clusters at finite temperature: Evidence for a noncyclic pentamer. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 15423-15428.	7.1	55
38	Exceptional Catalytic Nature of Quantum Dots for Photocatalytic Hydrogen Evolution without External Cocatalysts. Advanced Functional Materials, 2018, 28, 1801769.	14.9	54
39	Photoinduced Decomposition of Formaldehyde on a TiO <sub>2</sub> (110) Surface, Assisted by Bridge-Bonded Oxygen Atoms. Journal of Physical Chemistry Letters, 2013, 4, 2668-2673.	4.6	52
40	Quantum interference in H + HD $\hat{a}^{\dagger}$ H $\langle sub \rangle 2 \langle sub \rangle + D$ between direct abstraction and roaming insertion pathways. Science, 2020, 368, 767-771.	12.6	52
41	The vibrational distribution of the OH product from H2O photodissociation at 157 nm: Discrepancies between theory and experiment. Journal of Chemical Physics, 1999, 110, 4119-4122.	3.0	51
42	Infrared Spectroscopy of Neutral Water Dimer Based on a Tunable Vacuum Ultraviolet Free Electron Laser. Journal of Physical Chemistry Letters, 2020, 11, 851-855.	4.6	50
43	Stable Pt Single Atoms and Nanoclusters on Ultrathin CuO Film and Their Performances in CO Oxidation. Journal of Physical Chemistry C, 2016, 120, 1709-1715.	3.1	48
44	Effect of the Hydrogen Bond in Photoinduced Water Dissociation: A Double-Edged Sword. Journal of Physical Chemistry Letters, 2016, 7, 603-608.	4.6	46
45	Direct observation of forward-scattering oscillations in the H+HDâ†'H2+D reaction. Nature Chemistry, 2018, 10, 653-658.	13.6	46
46	Vacuum ultraviolet photochemistry of methane, silane and germane. Physical Chemistry Chemical Physics, 2001, 3, 1848-1860.	2.8	44
47	Effect of Surface Structure on the Photoreactivity of TiO <sub>2</sub> . Journal of Physical Chemistry C, 2015, 119, 6121-6127.	3.1	43
48	The Anion Effect on Li <sup>+</sup> Ion Coordination Structure in Ethylene Carbonate Solutions. Journal of Physical Chemistry Letters, 2016, 7, 3554-3559.	4.6	42
49	State-to-state dynamics of elementary chemical reactions using Rydberg H-atom translational spectroscopy. International Reviews in Physical Chemistry, 2005, 24, 37-98.	2.3	41
50	A kinetic study of the CH <sub>2</sub> OO Criegee intermediate reaction with SO <sub>2</sub> , (H <sub>2</sub> O) <sub>2</sub> , CH <sub>2</sub> I <sub>2</sub> and I atoms using OH laser induced fluorescence. Physical Chemistry Chemical Physics, 2017, 19, 20786-20794.	2.8	40
51	Role of Pt Loading in the Photocatalytic Chemistry of Methanol on Rutile TiO <sub>2</sub> (110). ACS Catalysis, 2019, 9, 286-294.	11.2	39
52	Ultrafast Transient Spectra and Dynamics of MXene (Ti <sub>3</sub> C <sub>2</sub> T <sub><i>x</i></sub> ) in Response to Light Excitations of Various Wavelengths. Journal of Physical Chemistry C, 2020, 124, 6441-6447.	3.1	39
53	Extremely Rotationally Excited OH from Water (HOD) Photodissociation through Conical Intersection. Physical Review Letters, 2001, 87, 253201.	7.8	38
54	Dynamical Resonances in the Fluorine Atom Reaction with the Hydrogen Molecule. Accounts of Chemical Research, 2008, 41, 981-989.	15.6	38

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55	Electronic structure and photoabsorption of Ti <sup>3+</sup> ions in reduced anatase and rutile TiO <sub>2</sub> . Physical Chemistry Chemical Physics, 2018, 20, 17658-17665.	2.8	38
56	Photodissociation dynamics of cyclopropane at 157 nm. Journal of Chemical Physics, 2002, 117, 153-160.	3.0	37
57	Multiple channel dynamics in the $O(1D)$ reaction with alkanes. Physical Chemistry Chemical Physics, 2006, 8, 205-215.	2.8	37
58	Photocatalytic Dissociation of Ethanol on TiO2(110) by Near-Band-Gap Excitation. Journal of Physical Chemistry C, 2013, 117, 10336-10344.	3.1	37
59	Direct Imaging Single Methanol Molecule Photocatalysis on Titania. Journal of Physical Chemistry C, 2015, 119, 17748-17754.	3.1	37
60	Hydroxyl super rotors from vacuum ultraviolet photodissociation of water. Nature Communications, 2019, 10, 1250.	12.8	37
61	Ultraviolet photolysis of H2S and its implications for SH radical production in the interstellar medium. Nature Communications, 2020, 11, 1547.	12.8	37
62	State to State to State Dynamics of the D+H2â†'HD+HReaction: Control of Transition-State Pathways via Reagent Orientation. Physical Review Letters, 2006, 96, 093201.	7.8	35
63	Highly Efficient Water Dissociation on Anatase TiO <sub>2</sub> (101). Journal of Physical Chemistry C, 2016, 120, 26807-26813.	3.1	35
64	Infrared spectroscopic study of hydrogen bonding topologies in the smallest ice cube. Nature Communications, 2020, 11, 5449.	12.8	35
65	Imaging CO $\langle$ sub $\rangle$ 2 $\langle$ sub $\rangle$ Photodissociation at 157 nm: State-to-State Correlations between CO( $\hat{1}$ $\frac{1}{2}$ ) and O( $\langle$ sup $\rangle$ 3 $\langle$ sup $\rangle$ P $\langle$ sub $\rangle$ 4 $\langle$ i $\rangle$ =0,1,2 $\langle$ sub $\rangle$ 0. Journal of Physical Chemistry Letters, 2010, 1, 1861-1865.	4.6	34
66	Dynamical resonances in chemical reactions. Chemical Society Reviews, 2018, 47, 6744-6763.	38.1	34
67	Enhanced reactivity of fluorine with para-hydrogen in cold interstellar clouds by resonance-induced quantum tunnelling. Nature Chemistry, $2019, 11, 744-749$ .	13.6	34
68	Effect of a Single Quantum Rotational Excitation on State-to-State Dynamics of theO(D1)+H2â†'OH+HReaction. Physical Review Letters, 2002, 89, 133201.	7.8	33
69	Tunable VUV photochemistry using Rydberg H-atom time-of-flight spectroscopy. Review of Scientific Instruments, 2008, 79, 124101.	1.3	33
70	Nonstatistical spin dynamics in photodissociation of H2O at 157nm. Journal of Chemical Physics, 2008, 128, 066101.	3.0	33
71	Mode specificity for the dissociative chemisorption of H <sub>2</sub> O on Cu(111): a quantum dynamics study on an accurately fitted potential energy surface. Physical Chemistry Chemical Physics, 2016, 18, 8537-8544.	2.8	33
72	Tunable VUV photochemistry using vacuum ultraviolet free electron laser combined with H-atom Rydberg tagging time-of-flight spectroscopy. Review of Scientific Instruments, 2018, 89, 063113.	1.3	33

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73	Elementary Chemical Reactions in Surface Photocatalysis. Annual Review of Physical Chemistry, 2018, 69, 451-472.	10.8	31
74	Probing Feshbach resonances in F+H2(j=1)â†'HF+H: Dynamical effect of single quantum H2-rotation. Journal of Chemical Physics, 2006, 125, 151102.	3.0	30
75	Observation of the geometric phase effect in the H+HDâ†'H2+D reaction below the conical intersection. Nature Communications, 2020, 11, 3640.	12.8	30
76	Flower-like cobalt carbide for efficient carbon dioxide conversion. Chemical Communications, 2020, 56, 7849-7852.	4.1	30
77	High resolution time-of-flight spectrometer for crossed molecular beam study of elementary chemical reactions. Review of Scientific Instruments, 2005, 76, 083107.	1.3	29
78	Selfâ€Assembled Amphiphilic Water Oxidation Catalysts: Control of Oâ^'O Bond Formation Pathways by Different Aggregation Patterns. Angewandte Chemie - International Edition, 2016, 55, 6229-6234.	13.8	29
79	Low-Temperature Hydrogen Production via Water Conversion on Pt/TiO <sub>2</sub> . Journal of Physical Chemistry C, 2018, 122, 10956-10962.	3.1	29
80	Photodissociation dynamics of H2O at 111.5 nm by a vacuum ultraviolet free electron laser. Journal of Chemical Physics, 2018, 148, 124301.	3.0	29
81	How Is Câ€"H Vibrational Energy Redistributed in F + CHD <sub>3</sub> (ν <sub>1</sub> = 1) ↠HF + CD <sub>3</sub> ?. Journal of Physical Chemistry Letters, 2014, 5, 1790-1794.	4.6	28
82	Photodissociation dynamics of H2O: Effect of unstable resonances on the \$ilde B, $^{1}$ {m !A}_{1}\$Bif1A1 electronic state. Journal of Chemical Physics, 2011, 134, 064301.	3.0	27
83	Surface photochemistry probed by two-photon photoemission spectroscopy. Energy and Environmental Science, 2012, 5, 6833.	30.8	27
84	Kinetics of the reaction of the simplest Criegee intermediate with ammonia: a combination of experiment and theory. Physical Chemistry Chemical Physics, 2018, 20, 29669-29676.	2.8	27
85	Transformation between the Dark and Bright Self-Trapped Excitons in Lead-Free Double-Perovskite Cs <sub>2</sub> NaBiCl <sub>6</sub> under Pressure. Journal of Physical Chemistry Letters, 2021, 12, 7285-7292.	4.6	27
86	Recombination of Formaldehyde and Hydrogen Atoms on TiO <sub>2</sub> (110). Journal of Physical Chemistry C, 2015, 119, 1170-1174.	3.1	26
87	Real-space imaging with pattern recognition of a ligand-protected Ag374 nanocluster at sub-molecular resolution. Nature Communications, 2018, 9, 2948.	12.8	26
88	Solvation structure around the Li <sup>+</sup> ion in succinonitrileâ€"lithium salt plastic crystalline electrolytes. Physical Chemistry Chemical Physics, 2016, 18, 14867-14873.	2.8	25
89	Unimolecular Reaction Rate Measurement of syn-CH3CHOO. Journal of Physical Chemistry Letters, 2019, 10, 4817-4821.	4.6	24
90	Two-photon photodissociation dynamics of H2O via the $\hat{DIf}$ electronic state. Journal of Chemical Physics, 2009, 131, 074301.	3.0	23

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91	VUV Photodissociation Dynamics of Nitrous Oxide: The O( $<$ sup $>$ 1 $<$ sup $>$ 5 $<$ sub $>$ (i $>$ 1 $<$ li>=0 $<$ sub $>$ ) and O( $<$ sup $>$ 9 $<$ sub $>$ 6 $>$ 1 $<$ 1 $>1>1<1>1>2>1>1>1>1>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>2>1>1>2>1>1>2>1>1>1>1>1>1>1>1>1>1>1>1>1>1>1>1>1>1>1$	2.5	22
92	Infrared-Vacuum Ultraviolet Spectroscopic and Theoretical Study of Neutral Methylamine Dimer. Journal of Physical Chemistry A, 2017, 121, 7176-7182.	2.5	21
93	Ordered-to-Disordered Transformation of Enhanced Water Structure on Hydrophobic Surfaces in Concentrated Alcohol–Water Solutions. Journal of Physical Chemistry Letters, 2019, 10, 7922-7928.	4.6	21
94	Velocity map imaging study of OCS photodissociation followed by $S(1S)$ autoionization at 157 nm. Molecular Physics, 2005, 103, 1797-1807.	1.7	20
95	Competition between Direct and Indirect Dissociation Pathways in Ultraviolet Photodissociation of HNCO. Journal of Physical Chemistry A, 2013, 117, 11673-11678.	2.5	20
96	Optimal d-band-induced Cu <sub>3</sub> N as a cocatalyst on metal sulfides for boosting photocatalytic hydrogen evolution. Journal of Materials Chemistry A, 2020, 8, 22601-22606.	10.3	20
97	Trapped Abstraction in the O( <sup>1</sup> D) + CHD <sub>3</sub> â†' OH + CD <sub>3</sub> Reaction. Journal of Physical Chemistry Letters, 2014, 5, 3106-3111.	4.6	19
98	Observation of the Carbon Elimination Channel in Vacuum Ultraviolet Photodissociation of OCS. Journal of Physical Chemistry Letters, 2019, 10, 4783-4787.	4.6	19
99	Infrared spectra of neutral dimethylamine clusters: An infrared-vacuum ultraviolet spectroscopic and anharmonic vibrational calculation study. Journal of Chemical Physics, 2019, 150, 064317.	3.0	19
100	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.	4.6	19
101	Reactivity oscillation in the heavy–light–heavy Cl + CH <sub>4</sub> reaction. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 9202-9207.	7.1	19
102	Surface Photocatalysis-TPD Spectrometer for Photochemical Kinetics. Chinese Journal of Chemical Physics, 2012, 25, 507-512.	1.3	18
103	Vibronically induced decay paths from the \$ilde C\$Clf1B1-state of water and its isotopomers. Journal of Chemical Physics, 2013, 138, 104306.	3.0	18
104	Imaging the Pair-Correlated HNCO Photodissociation: The NH( $\langle i\rangle a\langle  i\rangle \langle sup\rangle 1\langle  sup\rangle \hat{l}^*$ ) + CO(X $\langle sup\rangle 1\langle  sup\rangle \hat{l}^* \langle sup\rangle + \langle  sup\rangle \hat{l}^*$ ) Channel. Journal of Physical Chemistry A, 2014, 118, 2413-2418.	2.5	18
105	Charting a course for chemistry. Nature Chemistry, 2019, 11, 286-294.	13.6	18
106	Origin of the Adsorption-State-Dependent Photoactivity of Methanol on TiO <sub>2</sub> (110). ACS Catalysis, 2021, 11, 2620-2630.	11.2	18
107	Highly Rotationally Excited CH <sub>3</sub> from Methane Photodissociation through Conical Intersection Pathway. Journal of Physical Chemistry Letters, 2010, 1, 475-479.	4.6	17
108	Effect of CH stretching excitation on the reaction dynamics of F + CHD3 $\hat{a}^{\dagger}$ DF + CHD2. Journal of Chemical Physics, 2015, 143, 044316.	3.0	17

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109	Ultrafast Flash Energy Conductance at MXeneâ€Surfactant Interface and Its Molecular Origins. Advanced Materials Interfaces, 2019, 6, 1901461.	3.7	17
110	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.	4.6	17
111	Quantum interference between spin-orbit split partial waves in the F + HD → HF + D reaction. Science, 2021, 371, 936-940.	12.6	17
112	Alkoxylation Reaction of Alcohol on Silica Surfaces Studied by Sum Frequency Vibrational Spectroscopy. Journal of Physical Chemistry C, 2021, 125, 8638-8646.	3.1	17
113	Highly Efficient Pumping of Vibrationally Excited HD Molecules via Stark-Induced Adiabatic Raman Passage. Journal of Physical Chemistry Letters, 2013, 4, 368-371.	4.6	16
114	Photoinduced decomposition of acetaldehyde on a reduced TiO <sub>2</sub> (110) surface: involvement of lattice oxygen. Physical Chemistry Chemical Physics, 2016, 18, 30982-30989.	2.8	16
115	Photocatalytic chemistry of methanol on rutile TiO $<$ sub $>$ 2 $<$ /sub $>$ (011)-(2 $\tilde{A}-$ 1). Physical Chemistry Chemical Physics, 2016, 18, 10224-10231.	2.8	16
116	Li-lon solvation in propylene carbonate electrolytes determined by molecular rotational measurements. Physical Chemistry Chemical Physics, 2019, 21, 10417-10422.	2.8	16
117	Flexible high-resolution broadband sum-frequency generation vibrational spectroscopy for intrinsic spectral line widths. Journal of Chemical Physics, 2019, 150, 074702.	3.0	16
118	Probing state-to-state reaction dynamics using H-atom Rydberg tagging time-of-flight spectroscopy. Physical Chemistry Chemical Physics, 2011, 13, 8112.	2.8	15
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