

# Qijing Zheng

## List of Publications by Year in descending order

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42  
papers

1,864  
citations

304368

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276539

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42  
docs citations

42  
times ranked

1573  
citing authors

#	ARTICLE	IF	CITATIONS
1	Effects of oxygen vacancies on the photoexcited carrier lifetime in rutile TiO <sub>2</sub> . Physical Chemistry Chemical Physics, 2022, 24, 4743-4750.	1.3	8
2	Spin-orbit coupling induced demagnetization in Ni: <i>Ab initio</i> nonadiabatic molecular dynamics perspective. Physical Review B, 2022, 105, .	1.1	21
3	Excited electron and spin dynamics in topological insulator: A perspective from <i>ab initio</i> non-adiabatic molecular dynamics. Fundamental Research, 2022, 2, 506-510.	1.6	2
4	Ultrafast charge transfer coupled to quantum proton motion at molecule/metal oxide interface. Science Advances, 2022, 8, .	4.7	21
5	Dynamics of Photoexcited Small Polarons in Transition-Metal Oxides. Journal of Physical Chemistry Letters, 2021, 12, 2191-2198.	2.1	41
6	Real-time <i>GW</i> -BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide. Science Advances, 2021, 7, .	4.7	70
7	Strong Modulation of Band Gap, Carrier Mobility and Lifetime in Two-Dimensional Black Phosphorene through Acoustic Phonon Excitation. Journal of Physical Chemistry Letters, 2021, 12, 3960-3967.	2.1	30
8	Patterning of transition metal dichalcogenides catalyzed by surface plasmons with atomic precision. Chem, 2021, 7, 1626-1638.	5.8	11
9	Bidirectional and reversible tuning of the interlayer spacing of two-dimensional materials. Nature Communications, 2021, 12, 5886.	5.8	42
10	Phonon-phonon interaction assisted electron-hole recombination in WSe <sub>2</sub> /hBN van der Waals heterostructure. Journal of Applied Physics, 2021, 130, .	1.1	6
11	Ultrafast Ferroelectric Ordering on the Surface of a Topological Semimetal MoTe <sub>2</sub> . Nano Letters, 2021, 21, 9903-9908.	4.5	4
12	Time- and momentum-resolved image-potential states of 2H-MoS <sub>2</sub> surface. Physical Chemistry Chemical Physics, 2021, 23, 26336-26342.	1.3	1
13	Tuning the Lifetime of Photoexcited Small Polarons on Rutile TiO <sub>2</sub> Surface via Molecular Adsorption. Journal of Physical Chemistry C, 2021, 125, 27275-27282.	1.5	10
14	Tensile Strain-Controlled Photogenerated Carrier Dynamics at the van der Waals Heterostructure Interface. Journal of Physical Chemistry Letters, 2020, 11, 586-590.	2.1	41
15	Interfacial Hydrogen-Bonding Dynamics in Surface-Facilitated Dehydrogenation of Water on TiO <sub>2</sub> (110). Journal of the American Chemical Society, 2020, 142, 826-834.	6.6	31
16	Interlayer Polarization Explains Slow Charge Recombination in Two-Dimensional Halide Perovskites by Nonadiabatic Molecular Dynamics Simulation. Journal of Physical Chemistry Letters, 2020, 11, 9032-9037.	2.1	13
17	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2020, 11, 10073-10080.	2.1	65
18	Tuning the Carrier Lifetime in Black Phosphorene through Family Atom Doping. Journal of Physical Chemistry Letters, 2020, 11, 4662-4667.	2.1	48

#	ARTICLE	IF	CITATIONS
19	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. <i>Science Advances</i> , 2020, 6, eaaw7453.	4.7	182
20	CO <sub>2</sub> Photoreduction on Metal Oxide Surface Is Driven by Transient Capture of Hot Electrons: <i>Ab Initio</i> Quantum Dynamics Simulation. <i>Journal of the American Chemical Society</i> , 2020, 142, 3214-3221.	6.6	63
21	Ultrafast electron transfer dynamics in lateral transition-metal dichalcogenide heterostructures. <i>Electronic Structure</i> , 2019, 1, 034001.	1.0	9
22	Tailoring exciton dynamics of monolayer transition metal dichalcogenides by interfacial electron-phonon coupling. <i>Communications Physics</i> , 2019, 2, .	2.0	27
23	Suppression of Electron-Hole Recombination by Intrinsic Defects in 2D Monoelemental Material. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6151-6158.	2.1	62
24	Highly efficient photogenerated electron transfer at a black phosphorus/indium selenide heterostructure interface from ultrafast dynamics. <i>Journal of Materials Chemistry C</i> , 2019, 7, 1864-1870.	2.7	53
25	Photogenerated carrier dynamics at the anatase/rutile TiO <sub>2</sub> /H <sub>2</sub> O interface. <i>Physical Review B</i> , 2019, 99, .	1.1	22
26	Ab initio nonadiabatic molecular dynamics investigations on the excited carriers in condensed matter systems. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1411.	6.2	194
27	Diabatic Hamiltonian construction in van der Waals heterostructure complexes. <i>Journal of Materials Chemistry A</i> , 2019, 7, 27484-27492.	5.2	6
28	Dynamics of Single-Molecule Dissociation by Selective Excitation of Molecular Phonons. <i>Physical Review Letters</i> , 2019, 123, 246804.	2.9	4
29	Ultrafast dynamics of solvated electrons at anatase TiO <sub>2</sub> /H <sub>2</sub> O interface. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 114004.	0.7	5
30	Delocalized Impurity Phonon Induced Electron-Hole Recombination in Doped Semiconductors. <i>Nano Letters</i> , 2018, 18, 1592-1599.	4.5	86
31	Visualizing Elementary Reactions of Methanol by Electrons and Holes on TiO <sub>2</sub> (110) Surface. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28805-28814.	1.5	17
32	Direct Z-Scheme Water Splitting Photocatalyst Based on Two-Dimensional Van Der Waals Heterostructures. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5419-5424.	2.1	114
33	Phonon-coupled ultrafast interlayer charge oscillation at van der Waals heterostructure interfaces. <i>Physical Review B</i> , 2018, 97, .	1.1	81
34	Tuning Solvated Electrons by Polar Nonpolar Oxide Heterostructure. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3049-3056.	2.1	13
35	Superatom Molecular Orbital as an Interfacial Charge Separation State. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3485-3490.	2.1	29
36	<i>Ab initio</i> nonadiabatic molecular dynamics investigation on the dynamics of photogenerated spin hole current in Cu-doped MoS <sub>2</sub> . <i>Physical Review B</i> , 2017, 96, .	1.1	32

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37	Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface. <i>Nano Letters</i> , 2017, 17, 6435-6442.	4.5	204
38	Dynamic Equilibrium of Reversible Reactions and Migration of Hydrogen Atoms Mediated by Diffusive Methanol on Rutile TiO <sub>2</sub> (110)-(1 Å <sup>-1</sup> ) Surface. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7728-7735.	1.5	11
39	Ultrafast Dynamics of Photogenerated Holes at a CH <sub>3</sub> OH/TiO <sub>2</sub> Rutile Interface. <i>Journal of the American Chemical Society</i> , 2016, 138, 13740-13749.	6.6	126
40	Temperature- and Coverage-Dependent Kinetics of Photocatalytic Reaction of Methanol on TiO <sub>2</sub> (110)-(1 Å <sup>-1</sup> ) Surface. <i>Journal of Physical Chemistry C</i> , 2016, 120, 5503-5514.	1.5	43
41	Nonnuclear Nearly Free Electron Conduction Channels Induced by Doping Charge in Nanotube-Molecular Sheet Composites. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7255-7260.	1.1	14
42	High Photoreactivity on a Reconstructed Anatase TiO <sub>2</sub> (001) Surface Predicted by <i>Ab Initio</i> Nonadiabatic Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 0, , 5766-5775.	2.1	2