Qijing Zheng

List of Publications by Year in descending order

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42	1,864	304368	276539
papers	citations	22 h-index	41 g-index

42	42	42	1573
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface. Nano Letters, 2017, 17, 6435-6442.	4.5	204
2	Ab initio nonadiabatic molecular dynamics investigations on the excited carriers in condensed matter systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1411.	6.2	194
3	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. Science Advances, 2020, 6, eaaw7453.	4.7	182
4	Ultrafast Dynamics of Photongenerated Holes at a CH₃OH/TiO₂ Rutile Interface. Journal of the American Chemical Society, 2016, 138, 13740-13749.	6.6	126
5	Direct Z-Scheme Water Splitting Photocatalyst Based on Two-Dimensional Van Der Waals Heterostructures. Journal of Physical Chemistry Letters, 2018, 9, 5419-5424.	2.1	114
6	Delocalized Impurity Phonon Induced Electronâ€“Hole Recombination in Doped Semiconductors. Nano Letters, 2018, 18, 1592-1599.	4.5	86
7	Phonon-coupled ultrafast interlayer charge oscillation at van der Waals heterostructure interfaces. Physical Review B, 2018, 97, .	1.1	81
8	Real-time GW -BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide. Science Advances, 2021, 7, .	4.7	70
9	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2020, 11, 10073-10080.	2.1	65
10	CO₂ Photoreduction on Metal Oxide Surface Is Driven by Transient Capture of Hot Electrons: Ab Initio Quantum Dynamics Simulation. Journal of the American Chemical Society, 2020, 142, 3214-3221.	6.6	63
11	Suppression of Electronâ€“Hole Recombination by Intrinsic Defects in 2D Monoelemental Material. Journal of Physical Chemistry Letters, 2019, 10, 6151-6158.	2.1	62
12	Highly efficient photogenerated electron transfer at a black phosphorus/indium selenide heterostructure interface from ultrafast dynamics. Journal of Materials Chemistry C, 2019, 7, 1864-1870.	2.7	53
13	Tuning the Carrier Lifetime in Black Phosphorene through Family Atom Doping. Journal of Physical Chemistry Letters, 2020, 11, 4662-4667.	2.1	48
14	Temperature- and Coverage-Dependent Kinetics of Photocatalytic Reaction of Methanol on TiO₂ (110)-(1 Ã— 1) Surface. Journal of Physical Chemistry C, 2016, 120, 5503-5514.	1.5	43
15	Bidirectional and reversible tuning of the interlayer spacing of two-dimensional materials. Nature Communications, 2021, 12, 5886.	5.8	42
16	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
17	Dynamics of Photoexcited Small Polarons in Transition-Metal Oxides. Journal of Physical Chemistry Letters, 2021, 12, 2191-2198.	2.1	41
18	Ab initio nonadiabatic molecular dynamics investigation on the dynamics of photogenerated spin hole current in Cu-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2017, 96, .	1.1	32

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19	Interfacial Hydrogen-Bonding Dynamics in Surface-Facilitated Dehydrogenation of Water on TiO₂(110). Journal of the American Chemical Society, 2020, 142, 826-834.	6.6	31
20	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
21	Superatom Molecular Orbital as an Interfacial Charge Separation State. Journal of Physical Chemistry Letters, 2018, 9, 3485-3490.	2.1	29
22	Tailoring exciton dynamics of monolayer transition metal dichalcogenides by interfacial electron-phonon coupling. Communications Physics, 2019, 2, .	2.0	27
23	Photogenerated carrier dynamics at the anatase/rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> interface. Physical Review B, 2019, 99, .	1.1	22
24	Spin-orbit coupling induced demagnetization in Ni: Ab initio nonadiabatic molecular dynamics perspective. Physical Review B, 2022, 105, .	1.1	21
25	Ultrafast charge transfer coupled to quantum proton motion at molecule/metal oxide interface. Science Advances, 2022, 8, .	4.7	21
26	Visualizing Elementary Reactions of Methanol by Electrons and Holes on TiO₂(110) Surface. Journal of Physical Chemistry C, 2018, 122, 28805-28814.	1.5	17
27	Nonnuclear Nearly Free Electron Conduction Channels Induced by Doping Charge in Nanotubeâ€“Molecular Sheet Composites. Journal of Physical Chemistry A, 2014, 118, 7255-7260.	1.1	14
28	Tuning Solvated Electrons by Polarâ€“Nonpolar Oxide Heterostructure. Journal of Physical Chemistry Letters, 2018, 9, 3049-3056.	2.1	13
29	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
30	Dynamic Equilibrium of Reversible Reactions and Migration of Hydrogen Atoms Mediated by Diffusive Methanol on Rutile TiO₂ (110)-(1 Ã— 1) Surface. Journal of Physical Chemistry C, 2016, 120, 7728-7735.	1.5	11
31	Patterning of transition metal dichalcogenides catalyzed by surface plasmons with atomic precision. CheM, 2021, 7, 1626-1638.	5.8	11
32	Tuning the Lifetime of Photoexcited Small Polarons on Rutile TiO₂ Surface via Molecular Adsorption. Journal of Physical Chemistry C, 2021, 125, 27275-27282.	1.5	10
33	Ultrafast electron transfer dynamics in lateral transition-metal dichalcogenide heterostructures. Electronic Structure, 2019, 1, 034001.	1.0	9
34	Effects of oxygen vacancies on the photoexcited carrier lifetime in rutile TiO₂. Physical Chemistry Chemical Physics, 2022, 24, 4743-4750.	1.3	8
35	Diabatic Hamiltonian construction in van der Waals heterostructure complexes. Journal of Materials Chemistry A, 2019, 7, 27484-27492.	5.2	6
36	Phononâ€“phonon interaction assisted electronâ€“hole recombination in WSe2/hBN van der Waals heterostructure. Journal of Applied Physics, 2021, 130, .	1.1	6

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37	Ultrafast dynamics of solvated electrons at anatase TiO₂/H₂O interface. Journal of Physics Condensed Matter, 2019, 31, 114004.	0.7	5
38	Dynamics of Single-Molecule Dissociation by Selective Excitation of Molecular Phonons. Physical Review Letters, 2019, 123, 246804.	2.9	4
39	Ultrafast Ferroelectric Ordering on the Surface of a Topological Semimetal MoTe₂. Nano Letters, 2021, 21, 9903-9908.	4.5	4
40	Excited electron and spin dynamics in topological insulator: A perspective from ab initio non-adiabatic molecular dynamics. Fundamental Research, 2022, 2, 506-510.	1.6	2
41	High Photoreactivity on a Reconstructed Anatase TiO₂(001) Surface Predicted by Ab Initio Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry Letters, 0, , 5766-5775.	2.1	2
42	Time- and momentum-resolved image-potential states of 2H-MoS2 surface. Physical Chemistry Chemical Physics, 2021, 23, 26336-26342.	1.3	1