Zhen-Kun Tang

List of Publications by Year
in descending order

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70 papers	3,997 citations	147801 31 h-index	118850 62 g-index
72 all docs	72 docs citations	72 times ranked	6003 citing authors

#	Article	IF	Citations
1	Nonadiabatic Dynamics of Polaron Hopping and Coupling with Water on Reduced TiO₂. Journal of Physical Chemistry Letters, 2022, 13, 857-863.	4.6	6
2	The Role of Thermal Fluctuations and Vibrational Entropy: A Theoretical Insight into the Î´-to-Î± Transition of FAPbI₃. Journal of Physical Chemistry Letters, 2022, 13, 3089-3095.	4.6	5
3	How Hole Injection Accelerates Both Ion Migration and Nonradiative Recombination in Metal Halide Perovskites. Journal of the American Chemical Society, 2022, 144, 6604-6612.	13.7	31
4	Structure and Oxygen Evolution Activity of Î²-NiOOH: Where Are the Protons?. ACS Catalysis, 2022, 12, 295-304.	11.2	28
5	Realizing Two-Electron Transfer in Ni(OH)₂ Nanosheets for Energy Storage. Journal of the American Chemical Society, 2022, 144, 8969-8976.	13.7	116
6	The unique carrier mobility of Janus MoSSe/GaN heterostructures. Frontiers of Physics, 2021, 16, 1.	5.0	18
7	New Insight of Pyrroleâ€Like Nitrogen for Boosting Hydrogen Evolution Activity and Stability of Pt Single Atoms. Small, 2021, 17, e2004453.	10.0	38
8	Photoexcitation of bulk polarons in 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>. Physical Review B, 2021, 103, .	3.2	9
9	Amorphous Domains in Black Titanium Dioxide. Advanced Materials, 2021, 33, e2100407.	21.0	36
10	Recent advances in low-dimensional Janus materials: theoretical and simulation perspectives. Materials Advances, 2021, 2, 7543-7558.	5.4	38
11	Facet-Regulating Local Coordination of Dual-Atom Cocatalyzed TiO₂ for Photocatalytic Water Splitting. ACS Catalysis, 2021, 11, 14669-14676.	11.2	42
12	Subspace Occupancy-Constraining Potentials for Modeling Polaron Formation. Journal of Physical Chemistry C, 2021, 125, 26354-26362.	3.1	4
13	Valence oscillation and dynamic active sites in monolayer NiCo hydroxides for water oxidation. Nature Catalysis, 2021, 4, 1050-1058.	34.4	272
14	Realizing Fewâ€Layer Iodinene for Highâ€Rate Sodiumâ€Ion Batteries. Advanced Materials, 2020, 32, e2004835.	21.0	41
15	The oxygen vacancy in Li-ion battery cathode materials. Nanoscale Horizons, 2020, 5, 1453-1466.	8.0	77
16	Achieving delafossite analog by in situ electrochemical self-reconstruction as an oxygen-evolving catalyst. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 21906-21913.	7.1	67
17	Activity and selectivity of CO₂ photoreduction on catalytic materials. Dalton Transactions, 2020, 49, 12918-12928.	3.3	13
18	Water-Hydrogen-Polaron Coupling at Anatase TiO2(101) Surfaces: A Hybrid Density Functional Theory Study. Journal of Physical Chemistry Letters, 2020, 11, 4317-4325.	4.6	12

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19	Self-Induced Strain in 2D Chalcogenide Nanocrystals with Enhanced Photoelectrochemical Responsivity. Chemistry of Materials, 2020, 32, 2774-2781.	6.7	7
20	Theoretical Progress on the Relationship between the Structures and Properties of Perovskite Solar Cells. Advanced Theory and Simulations, 2020, 3, 2000022.	2.8	10
21	Synergy between Ion Migration and Charge Carrier Recombination in Metal-Halide Perovskites. Journal of the American Chemical Society, 2020, 142, 3060-3068.	13.7	91
22	The Electronic Structure and Optical Properties of Twoâ€Dimensional BiOXâ€“YO₃ (Xâ€‰=â€‰Cl, Br,) Tj ETQq0 0 0 rgBT	1.5	2
23	Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO₃ from First Principles. ACS Catalysis, 2019, 9, 10528-10535.	11.2	13
24	Atomic layer deposited Pt-Ru dual-metal dimers and identifying their active sites for hydrogen evolution reaction. Nature Communications, 2019, 10, 4936.	12.8	371
25	Structure and reactivity of highly reduced titanium oxide surface layers on TiO2: A first-principles study. Journal of Chemical Physics, 2019, 151, 184701.	3.0	7
26	Injection of oxygen vacancies in the bulk lattice of layered cathodes. Nature Nanotechnology, 2019, 14, 602-608.	31.5	321
27	The Influence of Dipole Moments Induced by Organic Molecules and Domain Structures on the Properties of CH₃NH₃PbI₃ Perovskite. Advanced Theory and Simulations, 2019, 2, 1900041.	2.8	5
28	Colloidal synthesis of SnS nanocrystals with dimension-dependent photoelectrochemical properties. New Journal of Chemistry, 2019, 43, 7457-7462.	2.8	15
29	New insights into interfacial photocharge transfer in TiO₂/C₃N₄ heterostructures: effects of facets and defects. New Journal of Chemistry, 2019, 43, 4511-4517.	2.8	27
30	Effect of Single-Atom Cocatalysts on the Activity of Faceted TiO₂ Photocatalysts. Langmuir, 2019, 35, 391-397.	3.5	54
31	InnenrÃ¼cktitelbild: Ice Melting to Release Reactants in Solution Syntheses (Angew. Chem. 13/2018). Angewandte Chemie, 2018, 130, 3579-3579.	2.0	1
32	Tuning defects in oxides at roomÂtemperature by lithium reduction. Nature Communications, 2018, 9, 1302.	12.8	428
33	Excess electrons in reduced rutile and anatase TiO2. Surface Science Reports, 2018, 73, 58-82.	7.2	106
34	Ice Melting to Release Reactants in Solution Syntheses. Angewandte Chemie - International Edition, 2018, 57, 3354-3359.	13.8	36
35	Ice Melting to Release Reactants in Solution Syntheses. Angewandte Chemie, 2018, 130, 3412-3417.	2.0	15
36	Tunable dipole and carrier mobility for a few layer Janus MoSSe structure. Journal of Materials Chemistry C, 2018, 6, 1693-1700.	5.5	164

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37	The effects of subsurface Ov and Tiint of anatase (1â€¯0â€¯1) surface on CO2 conversion: A first-principles study. Computational Materials Science, 2018, 155, 424-430.	3.0	8
38	Janus MoSSe Nanotubes: Tunable Band Gap and Excellent Optical Properties for Surface Photocatalysis. Advanced Theory and Simulations, 2018, 1, 1800082.	2.8	35
39	First-Principles Study of Novel Two-Dimensional (C₄H₉NH₃)₂PbX₄ Perovskites for Solar Cell Absorbers. Journal of Physical Chemistry Letters, 2017, 8, 876-883.	4.6	61
40	2D lateral heterostructures of monolayer and bilayer phosphorene. Journal of Materials Chemistry C, 2017, 5, 2291-2300.	5.5	25
41	Effect of water on the effective Goldschmidt tolerance factor and photoelectric conversion efficiency of organicâ€“inorganic perovskite: insights from first-principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 14955-14960.	2.8	10
42	Direct observation of multiple rotational stacking faults coexisting in freestanding bilayer MoS2. Scientific Reports, 2017, 7, 8323.	3.3	15
43	Enhanced optical absorption via cation doping hybrid lead iodine perovskites. Scientific Reports, 2017, 7, 7843.	3.3	61
44	Surface evolution of a Ptâ€“Pdâ€“Au electrocatalyst for stable oxygen reduction. Nature Energy, 2017, 2, .	39.5	302
45	Tuning band gaps and optical absorption of BiOCl through doping and strain: insight form DFT calculations. Physical Chemistry Chemical Physics, 2017, 19, 20968-20973.	2.8	34
46	The Effect of Excess Electron and hole on CO2 Adsorption and Activation on Rutile (110) surface. Scientific Reports, 2016, 6, 23298.	3.3	38
47	Unusual Li-Ion Transfer Mechanism in Liquid Electrolytes: A First-Principles Study. Journal of Physical Chemistry Letters, 2016, 7, 4795-4801.	4.6	39
48	Spatial separation of photo-generated electron-hole pairs in BiOBr/BiOI bilayer to facilitate water splitting. Scientific Reports, 2016, 6, 32764.	3.3	53
49	Electrocatalysis enhancement of iron-based catalysts induced by synergy of methanol and oxygen-containing groups. Nano Energy, 2016, 21, 265-275.	16.0	12
50	Hierarchical three-dimensional NiCo₂O₄ nanoneedle arrays supported on Ni foam for high-performance supercapacitors. RSC Advances, 2015, 5, 25304-25311.	3.6	67
51	CO₂ Capture and Conversion on Rutile TiO₂(110) in the Water Environment: Insight by First-Principles Calculations. Journal of Physical Chemistry Letters, 2015, 6, 2538-2545.	4.6	60
52	Two-dimensional square-pyramidal VO₂ with tunable electronic properties. Journal of Materials Chemistry C, 2015, 3, 3189-3197.	5.5	20
53	Uncovering the Veil of the Degradation in Perovskite CH₃NH₃PbI₃ upon Humidity Exposure: A First-Principles Study. Journal of Physical Chemistry Letters, 2015, 6, 3289-3295.	4.6	171
54	Effect of surface composition on electronic properties of methylammonium lead iodide perovskite. Journal of Materiomics, 2015, 1, 213-220.	5.7	49

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55	Stable ScS2 nanostructures with tunable electronic and magnetic properties. Solid State Communications, 2015, 220, 12-16.	1.9	12
56	Electronic and magnetism properties of two-dimensional stacked nickel hydroxides and nitrides. Scientific Reports, 2015, 5, 11656.	3.3	10
57	Two-dimensional hexagonal V₂O nanosheet and nanoribbons. Applied Physics Express, 2015, 8, 035201.	2.4	2
58	Tunable band gap and magnetism of the two-dimensional nickel hydroxide. RSC Advances, 2015, 5, 77154-77158.	3.6	24
59	Two-dimensional Ni(OH) ₂ -XS ₂ (X = Mo and W) heterostructures. 2D Materials, 2015, 2, 034014.	4.4	11
60	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. Physical Chemistry Chemical Physics, 2014, 16, 25854-25861.	2.8	105
61	New manifold two-dimensional single-layer structures of zinc-blende compounds. Journal of Materials Chemistry A, 2014, 2, 17971-17978.	10.3	107
62	A novel three dimensional semimetallic MoS2. Journal of Applied Physics, 2014, 115, .	2.5	6
63	The stability and electronic properties of novel three-dimensional graphene-MoS2 hybrid structure. Scientific Reports, 2014, 4, 7007.	3.3	45
64	Magnetic properties of a SnO2 quantum dot. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 53, 72-77.	2.7	9
65	Enhance ferromagnetism by stabilizing the cation vacancies in GaN. European Physical Journal B, 2013, 86, 1.	1.5	7
66	Electronic and magnetism properties of half-bare zigzag silicon carbon nanoribbons from hybrid density functional calculations. Solid State Communications, 2013, 158, 25-28.	1.9	7
67	Enhanced ferromagnetism by adding electrons in triple-decker Gdâ€“phthalocyanine. Physica Scripta, 2013, 87, 045701.	2.5	1
68	Shallow donor levels enhanced ferromagnetism in the In 2 O 3 :Co nanocrystal. Europhysics Letters, 2012, 97, 57006.	2.0	9
69	Ferromagnetic coupling in Mgâ€doped passivated AlN nanowires: A firstâ€principles study. Physica Status Solidi (B): Basic Research, 2012, 249, 185-189.	1.5	10
70	The role of permanent and induced electrostatic dipole moments for Schottky barriers in Janus MXY/graphene heterostructures: a first-principles study. Dalton Transactions, 0, , .	3.3	11