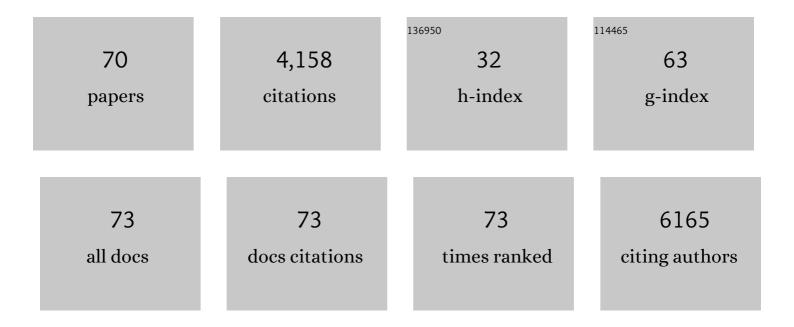
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Electric fields and substrates dramatically accelerate spin relaxation in graphene. Physical Review B, 2022, 105, .	3.2	4
2	Carbon trimer as a 2ÂeV single-photon emitter candidate in hexagonal boron nitride: A first-principles study. Physical Review Materials, 2022, 6, .	2.4	23
3	Room-temperature electrically switchable spin–valley coupling in a van der Waals ferroelectric halide perovskite with persistent spin helix. Nature Photonics, 2022, 16, 529-537.	31.4	35
4	Organically Capped Iridium Nanoparticles as High-Performance Bifunctional Electrocatalysts for Full Water Splitting in Both Acidic and Alkaline Media: Impacts of Metal–Ligand Interfacial Interactions. ACS Catalysis, 2021, 11, 1179-1188.	11.2	65
5	Interplay between Perovskite Magic-Sized Clusters and Amino Lead Halide Molecular Clusters. Research, 2021, 2021, 6047971.	5.7	13
6	High-order superlattices by rolling up van der Waals heterostructures. Nature, 2021, 591, 385-390.	27.8	163
7	Intersystem crossing and exciton–defect coupling of spin defects in hexagonal boron nitride. Npj Computational Materials, 2021, 7, .	8.7	24
8	Substrate effect on excitonic shift and radiative lifetime of two-dimensional materials. Journal of Physics Condensed Matter, 2021, 33, 234001.	1.8	9
9	Doping Bottleneck in Hematite: Multipole Clustering by Small Polarons. Chemistry of Materials, 2021, 33, 4390-4398.	6.7	22
10	Single-shot complete spatiotemporal measurement of terawatt laser pulses. Journal of Optics (United) Tj ETQqO	0 0 rgBT /( 2.2	Overlock 10 12
11	Enhancing Defect Tolerance with Ligands at the Surface of Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 6299-6304.	4.6	20
12	Computational design of quantum defects in two-dimensional materials. Nature Computational Science, 2021, 1, 646-654.	8.0	11
13	Giant Spin Lifetime Anisotropy and Spin-Valley Locking in Silicene and Germanene from First-Principles Density-Matrix Dynamics. Nano Letters, 2021, 21, 9594-9600.	9.1	7
14	<i>Ab initio</i> ultrafast spin dynamics in solids. Physical Review B, 2021, 104, .	3.2	10
15	Insights into the pH-dependent Behavior of N-Doped Carbons for the Oxygen Reduction Reaction by First-Principles Calculations. Journal of Physical Chemistry C, 2021, 125, 26429-26436.	3.1	3
16	Approaching the intrinsic exciton physics limit in two-dimensional semiconductor diodes. Nature, 2021, 599, 404-410.	27.8	57
17	The critical role of synthesis conditions on small polaron carrier concentrations in hematite—A first-principles study. Journal of Applied Physics, 2021, 130, .	2.5	4

18Interstitial Lithium Doping in BiVO<sub>4</sub> Thin Film Photoanode for Enhanced Solar Water<br/>Splitting Activity. Chemistry of Materials, 2020, 32, 6401-6409.6.737

#	Article	IF	CITATIONS
19	Development of high power laser platforms to study metal ejecta interactions. AIP Conference Proceedings, 2020, , .	0.4	7
20	Development of a Platform at the Matter in Extreme Conditions End Station for Characterization of Matter Heated by Intense Laser-Accelerated Protons. IEEE Transactions on Plasma Science, 2020, 48, 2751-2758.	1.3	4
21	Substrate screening approach for quasiparticle energies of two-dimensional interfaces with lattice mismatch. Physical Review B, 2020, 102, .	3.2	8
22	Spin-phonon relaxation from a universal ab initio density-matrix approach. Nature Communications, 2020, 11, 2780.	12.8	26
23	Electrochemical Oxidation of Metal–Catechol Complexes as a New Synthesis Route to the High-Quality Ternary Photoelectrodes: A Case Study of Fe <sub>2</sub> TiO <sub>5</sub> Photoanodes. ACS Applied Materials & Interfaces, 2020, 12, 29275-29284.	8.0	11
24	Carbon doping switching on the hydrogen adsorption activity of NiO for hydrogen evolution reaction. Nature Communications, 2020, 11, 590.	12.8	170
25	Combined Experimental and Theoretical Investigations of n-Type BiFeO <sub>3</sub> for Use as a Photoanode in a Photoelectrochemical Cell. Chemistry of Materials, 2020, 32, 3262-3270.	6.7	39
26	The coupling of experiments with density functional theory in the studies of the electrochemical hydrogen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 8783-8812.	10.3	33
27	High-volume and -adiabat capsule ("HVACâ€) ignition: Lowered fuel compression requirements using advanced Hohlraums. Physics of Plasmas, 2020, 27, 122708.	1.9	3
28	Plasmonics in argentene. Physical Review Materials, 2020, 4, .	2.4	15
29	Oxygen Reduction Reaction Catalyzed by Carbon-Supported Platinum Few-Atom Clusters: Significant Enhancement by Doping of Atomic Cobalt. Research, 2020, 2020, 9167829.	5.7	18
30	Ultra-high (>30%) coupling efficiency designs for demonstrating central hot-spot ignition on the National Ignition Facility using a Frustraum. Physics of Plasmas, 2019, 26, .	1.9	25
31	Combined Theoretical and Experimental Investigations of Atomic Doping To Enhance Photon Absorption and Carrier Transport of LaFeO <sub>3</sub> Photocathodes. Chemistry of Materials, 2019, 31, 5890-5899.	6.7	42
32	Heat-release equation of state and thermal conductivity of warm dense carbon by proton differential heating. Physical Review E, 2019, 100, 043204.	2.1	10
33	Carrier recombination mechanism at defects in wide band gap two-dimensional materials from first principles. Physical Review B, 2019, 100, .	3.2	22
34	Oxygen Reduction Reaction Catalyzed by Black-Phosphorus-Supported Metal Nanoparticles: Impacts of Interfacial Charge Transfer. ACS Applied Materials & Interfaces, 2019, 11, 24707-24714.	8.0	33
35	Dimensionality and anisotropicity dependence of radiative recombination in nanostructured phosphorene. Journal of Materials Chemistry C, 2019, 7, 12891-12897.	5.5	19
36	Ruthenium atomically dispersed in carbon outperforms platinum toward hydrogen evolution in alkaline media. Nature Communications, 2019, 10, 631.	12.8	423

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37	Optical absorption induced by small polaron formation in transition metal oxides: The case of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"&gt;<mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml: mathvariant="normal"&gt;O<mml:mn>4</mml:mn></mml: </mml:msub></mml:mrow>.</mml:math 	mn <b>₂3</b> k/mi	m <b>l:ເສຫ</b> >
38	Nanowrinkled Carbon Aerogels Embedded with FeNx Sites as Effective Oxygen Electrodes for Rechargeable Zinc-Air Battery. Research, 2019, 2019, 6813585.	5.7	29
39	Theoretical and Experimental Insight into the Effect of Nitrogen Doping on Hydrogen Evolution Activity of Ni <sub>3</sub> S <sub>2</sub> in Alkaline Medium. Advanced Energy Materials, 2018, 8, 1703538.	19.5	225
40	Combining Landau–Zener theory and kinetic Monte Carlo sampling for small polaron mobility of doped BiVO <sub>4</sub> from first-principles. Journal of Materials Chemistry A, 2018, 6, 20025-20036.	10.3	51
41	Mechanistic insights of enhanced spin polaron conduction in CuO through atomic doping. Npj Computational Materials, 2018, 4, .	8.7	18
42	Spin-optotronic Properties of Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 6103-6111.	4.6	22
43	Role of Point Defects in Enhancing the Conductivity of BiVO <sub>4</sub> . Chemistry of Materials, 2018, 30, 7793-7802.	6.7	71
44	Point of Anchor: Impacts on Interfacial Charge Transfer of Metal Oxide Nanoparticles. Journal of the American Chemical Society, 2018, 140, 15290-15299.	13.7	18
45	Unconventional Relation between Charge Transport and Photocurrent via Boosting Small Polaron Hopping for Photoelectrochemical Water Splitting. ACS Energy Letters, 2018, 3, 2232-2239.	17.4	61
46	Fundamental principles for calculating charged defect ionization energies in ultrathin two-dimensional materials. Physical Review Materials, 2018, 2, .	2.4	50
47	Modelling heterogeneous interfaces for solar water splitting. Nature Materials, 2017, 16, 401-408.	27.5	252
48	Nitrogen and Iron-Codoped Carbon Hollow Nanotubules as High-Performance Catalysts toward Oxygen Reduction Reaction: A Combined Experimental and Theoretical Study. Chemistry of Materials, 2017, 29, 5617-5628.	6.7	92
49	First-principles electrostatic potentials for reliable alignment at interfaces and defects. Journal of Chemical Physics, 2017, 146, 104109.	3.0	49
50	The Reaction Mechanism with Free Energy Barriers at Constant Potentials for the Oxygen Evolution Reaction at the IrO <sub>2</sub> (110) Surface. Journal of the American Chemical Society, 2017, 139, 149-155.	13.7	243
51	Hydrogen evolution reaction catalyzed by ruthenium ion-complexed graphitic carbon nitride nanosheets. Journal of Materials Chemistry A, 2017, 5, 18261-18269.	10.3	136
52	Effect of defects on the small polaron formation and transport properties of hematite from first-principles calculations. Journal of Physics Condensed Matter, 2017, 29, 394006.	1.8	35
53	First-principles engineering of charged defects for two-dimensional quantum technologies. Physical Review Materials, 2017, 1, .	2.4	64
54	Laser shock XAFS studies at OMEGA facility. High Pressure Research, 2016, 36, 303-314.	1.2	14

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55	Ultrafast probe using femtosecond electron pulses: real-time probing plasma dynamics. , 2015, , .		1
56	Simultaneous enhancements in photon absorption and charge transport of bismuth vanadate photoanodes for solar water splitting. Nature Communications, 2015, 6, 8769.	12.8	471
57	Solvation effects on the band edge positions of photocatalysts from first principles. Physical Chemistry Chemical Physics, 2015, 17, 30499-30509.	2.8	47
58	Optimizing the Band Edges of Tungsten Trioxide for Water Oxidation: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 6019-6028.	3.1	63
59	Dynamics of charge clouds ejected from laser-induced warm dense gold nanofilms. Physical Review E, 2014, 90, 041102.	2.1	1
60	Synthesis, photoelectrochemical properties, and first principles study of n-type CuW1â^'xMoxO4 electrodes showing enhanced visible light absorption. Energy and Environmental Science, 2013, 6, 2440.	30.8	65
61	Electronic excitations in light absorbers for photoelectrochemical energy conversion: first principles calculations based on many body perturbation theory. Chemical Society Reviews, 2013, 42, 2437.	38.1	157
62	Optical properties of tungsten trioxide from first-principles calculations. Physical Review B, 2013, 87, .	3.2	71
63	<i>Ab initio</i> calculations of absorption spectra of semiconducting nanowires within many-body perturbation theory. Physical Review B, 2012, 85, .	3.2	16
64	Ballistic electron transport in non-equilibrium warm dense gold. High Energy Density Physics, 2012, 8, 303-306.	1.5	22
65	Probing the warm dense copper nano-foil with ultrafast electron shadow imaging and deflectometry. High Energy Density Physics, 2012, 8, 298-302.	1.5	5
66	Tungsten Oxide Clathrates for Water Oxidation: A First Principles Study. Chemistry of Materials, 2012, 24, 4252-4260.	6.7	37
67	Thermally Stable N <sub>2</sub> -Intercalated WO <sub>3</sub> Photoanodes for Water Oxidation. Journal of the American Chemical Society, 2012, 134, 18318-18324.	13.7	126
68	Solution of the Bethe-Salpeter equation without empty electronic states: Application to the absorption spectra of bulk systems. Physical Review B, 2012, 85, .	3.2	49
69	Amplification of Ultrashort Laser Pulses by a Resonant Raman Scheme in a Gas-Jet Plasma. Physical Review Letters, 2004, 92, 175007.	7.8	123
70	Formation of periodic structures in a laser spark. Physics of Plasmas, 2001, 8, 4174-4179.	1.9	7