List of Publications by Year in descending order

63	6,679	186209 28	118793 62
papers	citations	h-index	g-index

65	65	65	5758
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	1T-MoS2 monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. Applied Surface Science, 2022, 584, 152537.	3.1	66
2	Selfâ€Optimizing Effect in Lithium Storage of GeO₂ Induced by Heterointerface Regulation. Small, 2022, 18, e2106067.	5.2	5
3	Potassium Storage Performance of UiO-66 Derivatives from First Principles Calculations. Journal of Physical Chemistry C, 2022, 126, 4286-4295.	1.5	5
4	Development of Strong Visibleâ€Lightâ€Absorbing Cyclometalated Iridium(III) Complexes for Robust and Efficient Lightâ€Driven Hydrogen Production. Chemistry - A European Journal, 2022, 28, .	1.7	16
5	DFT investigations of KTiOPO4M<i>x</i> (M = K, Na, and Li) anodes for alkali-ion battery. Journal of Chemical Physics, 2022, 156, .	1.2	6
6	Theoretical study on Y-doped Na₂ZrO₃ as a high-capacity Na-rich cathode material based on anionic redox. Physical Chemistry Chemical Physics, 2022, 24, 16183-16192.	1.3	7
7	Molecular Engineering of Robust Starburst-Based Organic Photosensitizers for Highly Efficient Photocatalytic Hydrogen Generation from Water. Chemistry of Materials, 2022, 34, 5522-5534.	3.2	7
8	Li₈MnO₆: A Novel Cathode Material with Only Anionic Redox. ACS Applied Materials & Interfaces, 2022, 14, 29832-29843.	4.0	2
9	Blue-AsP monolayer as a promising anode material for lithium- and sodium-ion batteries: a DFT study. Physical Chemistry Chemical Physics, 2021, 23, 5143-5151.	1.3	28
10	A New Candidate in Polyanionic Compounds for a Potassium-Ion Battery Cathode: KTiOPO₄. Journal of Physical Chemistry Letters, 2021, 12, 2721-2726.	2.1	23
11	UiO-66 Metalâ€“Organic Framework as an Anode for a Potassium-Ion Battery: Quantum Mechanical Analysis. Journal of Physical Chemistry C, 2021, 125, 9679-9687.	1.5	21
12	Easily fabricated HARCP/HAp photocatalyst for efficient and fast removal of tetracycline under natural sunlight. Chemical Engineering Journal, 2021, 412, 128620.	6.6	23
13	Discovery and characterization of a novel perylenephotoreductant for the activation of aryl halides. Journal of Catalysis, 2021, 399, 111-120.	3.1	5
14	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. Applied Surface Science, 2021, 563, 150269.	3.1	43
15	Anionic Oxygen Redox in the High-Lithium Material Li₈SnO₆. Chemistry of Materials, 2021, 33, 834-844.	3.2	10
16	Energy-Transfer-Mediated Photocatalysis by a Bioinspired Organic Perylenephotosensitizer HiBRCP. Journal of Organic Chemistry, 2021, 86, 15284-15297.	1.7	6
17	In Situ Confined Co5Ge3 Alloy Nanoparticles in Nitrogen-Doped Carbon Nanotubes for Boosting Lithium Storage. ACS Applied Materials & Interfaces, 2020, 12, 46247-46253.	4.0	11
18	Density Functional Theory Study of Single-Atom V, Nb, and Ta Catalysts on Graphene and Carbon Nitride for Selective Nitrogen Reduction. ACS Applied Nano Materials, 2020, 3, 5149-5159.	2.4	51

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19	Rational Design of Hierarchical SnS₂ Microspheres with S Vacancy for Enhanced Sodium Storage Performance. ACS Sustainable Chemistry and Engineering, 2020, 8, 9519-9525.	3.2	52
20	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 7031-7038.	1.5	13
21	Thiourea-based polyimide/RGO composite cathode: A comprehensive study of storage mechanism with alkali metal ions. Science China Materials, 2020, 63, 1929-1938.	3.5	13
22	Metalâ€"organic framework-derived hollow structure CoS₂/nitrogen-doped carbon spheres for high-performance lithium/sodium ion batteries. Chemical Communications, 2020, 56, 3951-3954.	2.2	35
23	Cercosporin-bioinspired photoreductive activation of aryl halides under mild conditions. Journal of Catalysis, 2019, 380, 1-8.	3.1	19
24	Safe, Lowâ€Cost, Fastâ€Kinetics and Lowâ€Strain Inorganicâ€Openâ€Framework Anode for Potassiumâ€Ion Batteries. Angewandte Chemie - International Edition, 2019, 58, 16474-16479.	7.2	56
25	Cercosporin-bioinspired selective photooxidation reactions under mild conditions. Green Chemistry, 2019, 21, 6073-6081.	4.6	41
26	Reversible conversion reaction of GeO₂ boosts lithium-ion storage <i>via</i> Fe doping. Journal of Materials Chemistry A, 2019, 7, 4574-4580.	5.2	34
27	Effective Electrochemical Charge Storage in the High-Lithium Compound Li₈ZrO₆. ACS Applied Energy Materials, 2019, 2, 1274-1287.	2.5	4
28	Theoretical Design of Layered AlGaS3 as a New Nonlinear Optical Material with a Strong Second Harmonic Generation Response. Crystal Growth and Design, 2019, 19, 1632-1639.	1.4	1
29	Hierarchical spheres constructed by ultrathin VS₂ nanosheets for sodium-ion batteries. Journal of Materials Chemistry A, 2019, 7, 3691-3696.	5.2	94
30	Phthalocyanine and Metal Phthalocyanines Adsorbed on Graphene: A Density Functional Study. Journal of Physical Chemistry C, 2019, 123, 16614-16620.	1.5	33
31	Whether Corrugated or Planar Vacancy Graphene-like Carbon Nitride (g-C₃N₄) Is More Effective for Nitrogen Reduction Reaction?. Journal of Physical Chemistry C, 2019, 123, 17296-17305.	1.5	46
32	Perylenequinonoid-Catalyzed [4 + 1] and [4 + 2] Annulations of Azoalkenes: Photocatalytic Access to 1,2,3-Thiadiazole/1,4,5,6-Tetrahydropyridazine Derivatives. Journal of Organic Chemistry, 2019, 84, 7711-7721.	1.7	40
33	Sulfur-Doped Anatase TiO₂ as an Anode for High-Performance Sodium-Ion Batteries. ACS Applied Energy Materials, 2019, 2, 3791-3797.	2.5	46
34	Nanocomposite of Mo₂N Quantum Dots@MoO₃@Nitrogen-Doped Carbon as a High-Performance Anode for Lithium-Ion Batteries. ACS Sustainable Chemistry and Engineering, 2019, 7, 10198-10206.	3.2	30
35	Perylenequinonoid-catalyzed photoredox activation for the direct arylation of (het)arenes with sunlight. Organic and Biomolecular Chemistry, 2019, 17, 4364-4369.	1.5	40
36	Toward an Accurate Description of Thermally Activated Delayed Fluorescence: Equal Importance of Electronic and Geometric Factors. Journal of Physical Chemistry C, 2019, 123, 13869-13876.	1.5	11

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37	Hierarchical Composite of Roseâ€Like VS₂@S/Nâ€Doped Carbon with Expanded (001) Planes for Superior Liâ€Ion Storage. Small, 2019, 15, e1903904.	5.2	64
38	Electronic Structure and Excited State Dynamics of TiO₂Nanowires. ACS Symposium Series, 2019, , 23-46.	0.5	0
39	Exploring the potentials of Ti₃N₂ and Ti₃N₂X₂ (X = O, F, OH) monolayers as anodes for Li or non-Li ion batteries from first-principles calculations. RSC Advances, 2019, 9, 40340-40347.	1.7	15
40	Computational prediction for oxidation and reduction potentials of organic molecules used in organic light-emitting diodes. Organic Electronics, 2019, 64, 216-222.	1.4	31
41	MnSb₂S₄ Monolayer as an Anode Material for Metal-Ion Batteries. Chemistry of Materials, 2018, 30, 3208-3214.	3.2	74
42	Indium selenide monolayer: a two-dimensional material with strong second harmonic generation. CrystEngComm, 2018, 20, 2573-2582.	1.3	16
43	Panchromatic Sensitization with Zn II Porphyrinâ€Based Photosensitizers for Lightâ€Driven Hydrogen Production. ChemSusChem, 2018, 11, 2517-2528.	3.6	30
44	Starburst Triarylamine Donor-Based Metal-Free Photosensitizers for Photocatalytic Hydrogen Production from Water. Organic Letters, 2017, 19, 1048-1051.	2.4	42
45	Localizing Holes as Polarons and Predicting Band Gaps, Defect Levels, and Delithiation Energies of Solid-State Materials with a Local Exchange-Correlation Functional. Journal of Physical Chemistry C, 2017, 121, 23955-23963.	1.5	18
46	Synthesis, structure, and photophysics of copper(<scp>i</scp>) triphenylphosphine complexes with functionalized 3-(2â€²-pyrimidinyl)-1,2,4-triazole ligands. Dalton Transactions, 2017, 46, 13077-13087.	1.6	30
47	Mechanism of electrochemical lithiation of a metal-organic framework without redox-active nodes. Journal of Chemical Physics, 2016, 144, 194702.	1.2	41
48	Conduction and Surface Effects in Cathode Materials: Li₈ZrO₆ and Doped Li₈ZrO₆. Journal of Physical Chemistry C, 2016, 120, 9637-9649.	1.5	14
49	Dynamics of charge at water-to-semiconductor interface: Case study of wet [0 0 1] anatase TiO2 nanowire. Chemical Physics, 2016, 481, 184-190.	0.9	5
50	Large-scale preparation of heterometallic chalcogenide MnSb₂S₄monolayer nanosheets with a high visible-light photocatalytic activity for H₂evolution. Chemical Communications, 2016, 52, 13381-13384.	2.2	18
51	Transition-Metal-Doped M-Li₈ZrO₆ (M = Mn, Fe, Co, Ni, Cu, Ce) as High-Specific-Capacity Li-Ion Battery Cathode Materials: Synthesis, Electrochemistry, and Quantum Mechanical Characterization. Chemistry of Materials, 2016, 28, 746-755.	3.2	30
52	Y-doped Li₈ZrO₆: A Li-Ion Battery Cathode Material with High Capacity. Journal of the American Chemical Society, 2015, 137, 10992-11003.	6.6	54
53	Anthraquinone-Based Intramolecular Charge-Transfer Compounds: Computational Molecular Design, Thermally Activated Delayed Fluorescence, and Highly Efficient Red Electroluminescence. Journal of the American Chemical Society, 2014, 136, 18070-18081.	6.6	822
54	Anatase TiO2 Nanowires, Thin Films, and Surfaces: Ab initio Studies of Electronic Properties and Non-adiabatic Excited State Dynamics. Materials Research Society Symposia Proceedings, 2014, 1659, 129-134.	0.1	3

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55	High-efficiency deep-blue organic light-emitting diodes based on a thermally activated delayed fluorescence emitter. Journal of Materials Chemistry C, 2014, 2, 421-424.	2.7	259
56	Electronic structure and hot carrier relaxation in âŸ¨001âŸ© anatase TiO₂nanowire. Molecular Physics, 2014, 112, 539-545.	0.8	17
57	Excited State Dynamics of Ru₁₀ Cluster Interfacing Anatase TiO₂(101) Surface and Liquid Water. Journal of Physical Chemistry Letters, 2014, 5, 2823-2829.	2.1	28
58	Charge Transfer, Luminescence, and Phonon Bottleneck in TiO₂ Nanowires Computed by Eigenvectors of Liouville Superoperator. Journal of Chemical Theory and Computation, 2014, 10, 3996-4005.	2.3	26
59	Efficient blue organic light-emitting diodes employing thermally activated delayed fluorescence. Nature Photonics, 2014, 8, 326-332.	15.6	2,064
60	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. Journal of Chemical Theory and Computation, 2013, 9, 3872-3877.	2.3	312
61	Design of Efficient Thermally Activated Delayed Fluorescence Materials for Pure Blue Organic Light Emitting Diodes. Journal of the American Chemical Society, 2012, 134, 14706-14709.	6.6	1,370
62	Triplet Exciton Confinement in Green Organic Lightâ€Emitting Diodes Containing Luminescent Chargeâ€Transfer Cu(I) Complexes. Advanced Functional Materials, 2012, 22, 2327-2336.	7.8	279
63	Moleculeâ€“substrate interaction channels of metal-phthalocyanines on graphene on Ni(111) surface. Journal of Chemical Physics, 2011, 134, 094705.	1.2	74