Yi Li

List of Publications by Year
in descending order

		430754	414303
43	1,116	18	32
papers	citations	h-index	g-index

43	43	43	1572
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Copper-on-nitride enhances the stable electrosynthesis of multi-carbon products from CO2. Nature Communications, 2018, 9, 3828.	5.8	279
2	MnSb₂S₄ Monolayer as an Anode Material for Metal-Ion Batteries. Chemistry of Materials, 2018, 30, 3208-3214.	3.2	74
3	Computational design of inorganic nonlinear optical crystals based on a genetic algorithm. CrystEngComm, 2014, 16, 10569-10580.	1.3	67
4	A Highly Effective Ï€â€“Ï€ Stacking Strategy To Modify Black Phosphorus with Aromatic Molecules for Cancer Theranostics. ACS Applied Materials & Interfaces, 2019, 11, 9860-9871.	4.0	47
5	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. Applied Surface Science, 2021, 563, 150269.	3.1	43
6	First-principles investigation of the activation of CO2 molecule on TM/Cu (TM=Fe, Co and Ni) surface alloys. Applied Surface Science, 2015, 353, 902-912.	3.1	38
7	Effects of ligand functionalization on the photocatalytic properties of titanium-based MOF: A density functional theory study. AIP Advances, 2018, 8, .	0.6	35
8	Structural and Electronic Properties of a W₃O₉Cluster Supported on the TiO₂(110) Surface. Journal of Physical Chemistry C, 2009, 113, 17509-17517.	1.5	34
9	What Is the Best Size of Subnanometer Copper Clusters for CO₂ Conversion to Methanol at Cu/TiO₂ Interfaces? A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 24118-24132.	1.5	32
10	Unraveling the mechanisms of S-doped carbon nitride for photocatalytic oxygen reduction to H₂O₂. Physical Chemistry Chemical Physics, 2020, 22, 21099-21107.	1.3	29
11	Effects of doping high-valence transition metal (V, Nb and Zr) ions on the structure and electrochemical performance of LIB cathode material LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂. Physical Chemistry Chemical Physics, 2021, 23, 11528-11537.	1.3	29
12	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
13	Electrocatalytic Nitrogen Reduction by Transition Metal Single-Atom Catalysts on Polymeric Carbon Nitride. Journal of Physical Chemistry C, 2021, 125, 13880-13888.	1.5	28
14	Nitrogen fixation on metal-free SiC(111) polar surfaces. Journal of Materials Chemistry A, 2020, 8, 7412-7421.	5.2	26
15	Lead-carboxylate/polyiodide hybrids constructed from halogen bonding and asymmetric viologen: structures, visible-light-driven photocatalytic properties and enhanced photocurrent responses. CrystEngComm, 2018, 20, 2245-2252.	1.3	25
16	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
17	Toward improving CO2 dissociation and conversion to methanol via CO-hydrogenation on Cu(100) surface by introducing embedded Co nanoclusters as promoters: A DFT study. Applied Surface Science, 2018, 427, 837-847.	3.1	22
18	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

#	Article	IF	Citations
19	Quaternary Phosphorusâ€Induced Iodocuprate(I)â€Based Hybrids: Water Stabilities, Tunable Luminescence and Photocurrent Responses. European Journal of Inorganic Chemistry, 2018, 2018, 4234-4244.	1.0	18
20	A boron-decorated melon-based carbon nitride as a metal-free photocatalyst for N₂ fixation: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 21872-21880.	1.3	18
21	Indium selenide monolayer: a two-dimensional material with strong second harmonic generation. CrystEngComm, 2018, 20, 2573-2582.	1.3	16
22	Combination of N-Arylstilbazolium Organic Nonlinear Optical Chromophores with Iodoargentates: Structural Diversities and Optical Properties. Crystal Growth and Design, 2018, 18, 3827-3840.	1.4	15
23	Exfoliation of transition-metal dichalcogenides using ATP in aqueous solution. Chemical Communications, 2019, 55, 2972-2975.	2.2	15
24	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
25	Defective BC₂N as an Anode Material with Improved Performance for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 4946-4954.	1.5	15
26	Insight into the mechanism for the methanol synthesis via the hydrogenation of CO2 over a Co-modified Cu(100) surface: A DFT study. Journal of Chemical Physics, 2016, 145, 134701.	1.2	14
27	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 7031-7038.	1.5	13
28	Two-Dimensional Silver-Thiocyanate Layers Directed by Viologens: Structural Transformations upon Low Pressure Stimuli, Piezochromic Luminescence, Photocurrent Responses, and Photocatalytic Properties. Crystal Growth and Design, 2019, 19, 177-192.	1.4	11
29	Pressure-tuning the nonlinear-optical properties of AgGaS_2 crystal: a first-principle study. Optical Materials Express, 2015, 5, 1738.	1.6	10
30	Tailoring the Linear and Second-Order Nonlinear Optical Responses of the Titanium-MIL-125 Metalâ€“Organic Framework through Ligand Functionalization: A First Principles Study. Journal of Physical Chemistry C, 2019, 123, 653-664.	1.5	9
31	Investigation of Ordered TiMC and TiMCT₂ (M = Cr and Mo; T = O and S) MXenes as High-Performance Anode Materials for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2022, 126, 5283-5291.	1.5	9
32	The mechanism for CO2 reduction over Fe-modified Cu(100) surfaces with thermodynamics and kinetics: a DFT study. RSC Advances, 2020, 10, 32569-32580.	1.7	7
33	Electronic Structures and Optical Properties of Organic DAST and DSTMS Crystal Materials. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2013, 29, 2534-2542.	2.2	6
34	Unveiling the Selectivity of CO₂ Reduction on Cu₂ZnSnS₄: The Effect of Exposed Termination. Journal of Physical Chemistry C, 2021, 125, 24967-24973.	1.5	6
35	Validation of Density Functional Theory Methods for Predicting the Optical Properties of Cu-Based Multinary Chalcogenide Semiconductors. Journal of Physical Chemistry C, 2022, 126, 4684-4697.	1.5	6
36	DFT investigations of KTiOPO4Mx (M = K, Na, and Li) anodes for alkali-ion battery. Journal of Chemical Physics, 2022, 156, .	1.2	6

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37	Microscopic functionality of FeN4 sites in polymeric carbon nitride for efficient H2S oxidation. Applied Surface Science, 2022, 600, 154011.	3.1	6
38	Understanding the Role of Various Dopant Metals (Sb, Sn, Ga, Ge, and V) in the Structural and Electrochemical Performances of LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂. Journal of Physical Chemistry C, 2021, 125, 19600-19608.	1.5	5
39	Potassium Storage Performance of UiO-66 Derivatives from First Principles Calculations. Journal of Physical Chemistry C, 2022, 126, 4286-4295.	1.5	5
40	Multifunctional Quaternary Phosphorus/Bromoargentate Hybrids: The Achievement of Greenish Blue Luminescence, Repeatable Photocurrent Responses and Durable Antimicrobial Activities with Enhanced Water Stability . International Journal of Nanomedicine, 2020, Volume 15, 6225-6237.	3.3	4
41	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO2 Activation. ACS Omega, 2021, 6, 27259-27270.	1.6	4
42	Novel luminescent homo/heterometallic platinum(ii) alkynyl complexes based on Y-shaped pyridyl diphosphines. Dalton Transactions, 2020, 49, 8347-8353.	1.6	2
43	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