

Yi Li

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

41
papers

609
citations

13
h-index

24
g-index

43
ext. papers

858
ext. citations

4.7
avg, IF

3.95
L-index

#	Paper	IF	Citations
41	Potassium Storage Performance of UiO-66 Derivatives from First Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 4286-4295	3.8	1
40	Validation of Density Functional Theory Methods for Predicting the Optical Properties of Cu-Based Multinary Chalcogenide Semiconductors. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 4684-4697	3.8	0
39	Investigation of Ordered TiMC and TiMCT2 (M = Cr and Mo; T = O and S) MXenes as High-Performance Anode Materials for Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 5283-5291	3.8	0
38	Unveiling the Selectivity of CO ₂ Reduction on Cu ₂ ZnSnS ₄ : The Effect of Exposed Termination. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 24967-24973	3.8	3
37	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO Activation. <i>ACS Omega</i> , 2021 , 6, 27259-27270	3.9	0
36	A New Candidate in Polyanionic Compounds for a Potassium-Ion Battery Cathode: KTiOPO. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 2721-2726	6.4	6
35	Defective BC ₂ N as an Anode Material with Improved Performance for Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 4946-4954	3.8	4
34	UiO-66 Metal-Organic Framework as an Anode for a Potassium-Ion Battery: Quantum Mechanical Analysis. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 9679-9687	3.8	4
33	Electrocatalytic Nitrogen Reduction by Transition Metal Single-Atom Catalysts on Polymeric Carbon Nitride. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 13880-13888	3.8	7
32	Blue-AsP monolayer as a promising anode material for lithium- and sodium-ion batteries: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 5143-5151	3.6	7
31	Effects of doping high-valence transition metal (V, Nb and Zr) ions on the structure and electrochemical performance of LIB cathode material LiNiCoMnO. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 11528-11537	3.6	7
30	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} O ₂ . <i>Journal of Physical Chemistry C</i> , 2021 , 125, 19600-19608	3.8	3
29	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. <i>Applied Surface Science</i> , 2021 , 563, 150269	6.7	11
28	Novel luminescent homo/heterometallic platinum(ii) alkynyl complexes based on Y-shaped pyridyl diphosphines. <i>Dalton Transactions</i> , 2020 , 49, 8347-8353	4.3	0
27	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7031-7038	3.8	11
26	Nitrogen fixation on metal-free SiC(111) polar surfaces. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 7412-7421	4.9	17
25	A boron-decorated melon-based carbon nitride as a metal-free photocatalyst for N fixation: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 21872-21880	3.6	9

24	The mechanism for CO reduction over Fe-modified Cu(100) surfaces with thermodynamics and kinetics: a DFT study.. <i>RSC Advances</i> , 2020 , 10, 32569-32580	3.7	2
23	Multifunctional Quaternary Phosphorus/Bromoargentate Hybrids: The Achievement of Greenish Blue Luminescence, Repeatable Photocurrent Responses and Durable Antimicrobial Activities with Enhanced Water Stability. <i>International Journal of Nanomedicine</i> , 2020 , 15, 6225-6237	7.3	1
22	Unraveling the mechanisms of S-doped carbon nitride for photocatalytic oxygen reduction to HO. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 21099-21107	3.6	7
21	What Is the Best Size of Subnanometer Copper Clusters for CO ₂ Conversion to Methanol at Cu/TiO ₂ Interfaces? A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 24118-24132 ¹³	3.8	13
20	Theoretical Design of Layered AlGaS ₃ as a New Nonlinear Optical Material with a Strong Second Harmonic Generation Response. <i>Crystal Growth and Design</i> , 2019 , 19, 1632-1639	3.5	1
19	Exfoliation of transition-metal dichalcogenides using ATP in aqueous solution. <i>Chemical Communications</i> , 2019 , 55, 2972-2975	5.8	8
18	A Highly Effective π-Stacking Strategy To Modify Black Phosphorus with Aromatic Molecules for Cancer Theranostics. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 9860-9871	9.5	33
17	Exploring the potentials of TiN and TiNX (X = O, F, OH) monolayers as anodes for Li or non-Li ion batteries from first-principles calculations.. <i>RSC Advances</i> , 2019 , 9, 40340-40347	3.7	7
16	Tailoring the Linear and Second-Order Nonlinear Optical Responses of the Titanium-MIL-125 Metal-Organic Framework through Ligand Functionalization: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 653-664	3.8	7
15	Two-Dimensional Silver-Thiocyanate Layers Directed by Viologens: Structural Transformations upon Low Pressure Stimuli, Piezochromic Luminescence, Photocurrent Responses, and Photocatalytic Properties. <i>Crystal Growth and Design</i> , 2019 , 19, 177-192	3.5	8
14	MnSb ₂ S ₄ Monolayer as an Anode Material for Metal-Ion Batteries. <i>Chemistry of Materials</i> , 2018 , 30, 3208-3214 ³⁸	3.2	38
13	Effects of ligand functionalization on the photocatalytic properties of titanium-based MOF: A density functional theory study. <i>AIP Advances</i> , 2018 , 8, 035012	1.5	24
12	Lead-carboxylate/polyiodide hybrids constructed from halogen bonding and asymmetric viologen: structures, visible-light-driven photocatalytic properties and enhanced photocurrent responses. <i>CrystEngComm</i> , 2018 , 20, 2245-2252	3.3	22
11	Indium selenide monolayer: a two-dimensional material with strong second harmonic generation. <i>CrystEngComm</i> , 2018 , 20, 2573-2582	3.3	14
10	Toward improving CO ₂ dissociation and conversion to methanol via CO-hydrogenation on Cu(100) surface by introducing embedded Co nanoclusters as promoters: A DFT study. <i>Applied Surface Science</i> , 2018 , 427, 837-847	6.7	16
9	Quaternary Phosphorus-Induced Iodocuprate(I)-Based Hybrids: Water Stabilities, Tunable Luminescence and Photocurrent Responses. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 4234-4244 ²³	2.3	9
8	Copper-on-nitride enhances the stable electrosynthesis of multi-carbon products from CO. <i>Nature Communications</i> , 2018 , 9, 3828	17.4	164
7	Combination of N-Arylstilbazolium Organic Nonlinear Optical Chromophores with Iodoargentates: Structural Diversities and Optical Properties. <i>Crystal Growth and Design</i> , 2018 , 18, 3827-3840	3.5	14

6	Insight into the mechanism for the methanol synthesis via the hydrogenation of CO over a Co-modified Cu(100) surface: A DFT study. <i>Journal of Chemical Physics</i> , 2016 , 145, 134701	3.9	12
5	First-principles investigation of the activation of CO ₂ molecule on TM/Cu (TM = Fe, Co and Ni) surface alloys. <i>Applied Surface Science</i> , 2015 , 353, 902-912	6.7	24
4	Pressure-tuning the nonlinear-optical properties of AgGaS ₂ crystal: a first-principle study. <i>Optical Materials Express</i> , 2015 , 5, 1738	2.6	9
3	Computational design of inorganic nonlinear optical crystals based on a genetic algorithm. <i>CrystEngComm</i> , 2014 , 16, 10569-10580	3.3	49
2	Electronic Structures and Optical Properties of Organic DAST and DSTMS Crystal Materials. <i>Wuli Huaxue Xuebao/Acta Physico - Chimica Sinica</i> , 2013 , 29, 2534-2542	3.8	4
1	Structural and Electronic Properties of a W ₃ O ₉ Cluster Supported on the TiO ₂ (110) Surface. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 17509-17517	3.8	32