Yu Qie

List of Publications by Year
in descending order

68	4,913	147566	110170
papers	citations	31 h-index	64 g-index

69	69	69	5196
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Clustering of Ti on a C60Surface and Its Effect on Hydrogen Storage. Journal of the American Chemical Society, 2005, 127, 14582-14583.	6.6	675
2	Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. Chemical Reviews, 2018, 118, 5755-5870.	23.0	426
3	Lithium Chlorides and Bromides as Promising Solidâ€State Chemistries for Fast Ion Conductors with Good Electrochemical Stability. Angewandte Chemie - International Edition, 2019, 58, 8039-8043.	7.2	322
4	Recent Advances in Breaking Scaling Relations for Effective Electrochemical Conversion of CO₂. Advanced Energy Materials, 2016, 6, 1600463.	10.2	308
5	Electronic and magnetic properties of a BN sheet decorated with hydrogen and fluorine. Physical Review B, 2010, 81, .	1.1	278
6	Solid Oxide Fuel Cell Anode Materials for Direct Hydrocarbon Utilization. Advanced Energy Materials, 2012, 2, 1156-1181.	10.2	253
7	CO₂ Electroreduction Performance of Transition Metal Dimers Supported on Graphene: A Theoretical Study. ACS Catalysis, 2015, 5, 6658-6664.	5.5	227
8	Electronic structures and bonding of graphyne sheet and its BN analog. Journal of Chemical Physics, 2011, 134, 174701.	1.2	182
9	Functionalized Graphitic Carbon Nitride for Efficient Energy Storage. Journal of Physical Chemistry C, 2013, 117, 6055-6059.	1.5	171
10	Theoretical Study of Hydrogen Storage in Ca-Coated Fullerenes. Journal of Chemical Theory and Computation, 2009, 5, 374-379.	2.3	130
11	All-carbon-based porous topological semimetal for Li-ion battery anode material. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 651-656.	3.3	125
12	Curvature-Dependent Selectivity of CO₂ Electrocatalytic Reduction on Cobalt Porphyrin Nanotubes. ACS Catalysis, 2016, 6, 6294-6301.	5.5	113
13	Interactions of Au cluster anions with oxygen. Journal of Chemical Physics, 2004, 120, 6510-6515.	1.2	107
14	Storage of Molecular Hydrogen in Bâ˜N Cage:â€‰ Energetics and Thermal Stability. Nano Letters, 2005, 5, 1273-1277.	4.5	106
15	C3B monolayer as an anchoring material for lithium-sulfur batteries. Carbon, 2018, 129, 38-44.	5.4	105
16	A Honeycomb BeN₂ Sheet with a Desirable Direct Band Gap and High Carrier Mobility. Journal of Physical Chemistry Letters, 2016, 7, 2664-2670.	2.1	100
17	CO₂ Electroreduction Performance of Phthalocyanine Sheet with Mn Dimer: A Theoretical Study. Journal of Physical Chemistry C, 2017, 121, 3963-3969.	1.5	95
18	Functionalized heterofullerenes for hydrogen storage. Applied Physics Letters, 2009, 94, .	1.5	89

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19	Tetragonal C₂₄: a topological nodal-surface semimetal with potential as an anode material for sodium ion batteries. Journal of Materials Chemistry A, 2019, 7, 5733-5739.	5.2	72
20	Energetics and local spin magnetic moment of single3,4dimpurities encapsulated in an icosahedralAu12cage. Physical Review B, 2004, 70, .	1.1	69
21	Valley-Polarized Quantum Anomalous Hall Effect in Ferrimagnetic Honeycomb Lattices. Physical Review Letters, 2017, 119, 046403.	2.9	64
22	Cu atomic chains supported on Î²-borophene sheets for effective CO₂electroreduction. Nanoscale, 2018, 10, 11064-11071.	2.8	50
23	Yttriumâ€“Sodium Halides as Promising Solid-State Electrolytes with High Ionic Conductivity and Stability for Na-Ion Batteries. Journal of Physical Chemistry Letters, 2020, 11, 3376-3383.	2.1	43
24	Boron-graphdiyne as an anode material for Li, Na, and K ion batteries with high capacities and low diffusion barriers. Journal of Renewable and Sustainable Energy, 2019, 11, .	0.8	42
25	Intrinsic ferromagnetism in two-dimensional carbon structures: Triangular graphene nanoflakes linked by carbon chains. Physical Review B, 2011, 84, .	1.1	40
26	Design of tetracene-based metallic 2D carbon materials for Na- and K-Ion batteries. Applied Surface Science, 2020, 521, 146456.	3.1	40
27	Enhanced Hydrogen Storage on Li Functionalized BC₃ Nanotube. Journal of Physical Chemistry C, 2011, 115, 6136-6140.	1.5	38
28	Topological semimetal porous carbon as a high-performance anode for Li-ion batteries. Journal of Materials Chemistry A, 2019, 7, 14253-14259.	5.2	36
29	Enhanced CO2 electroreduction on armchair graphene nanoribbons edge-decorated with copper. Nano Research, 2017, 10, 1641-1650.	5.8	35
30	Sc-phthalocyanine sheet: Promising material for hydrogen storage. Applied Physics Letters, 2011, 99, .	1.5	32
31	Recent advances in hybrid grapheneâ€BN planar structures. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 65-82.	6.2	32
32	High-pressure-assisted design of porous topological semimetal carbon for Li-ion battery anode with high-rate performance. Physical Review Materials, 2018, 2, .	0.9	32
33	Assembling biphenylene into 3D porous metallic carbon allotrope for promising anode of lithium-ion batteries. Carbon, 2022, 188, 95-103.	5.4	31
34	PCF-Graphene: A 2D sp²-Hybridized Carbon Allotrope with a Direct Band Gap. Journal of Physical Chemistry C, 2019, 123, 4567-4573.	1.5	29
35	Three-dimensional porous phosphorus-graphdiyne as a universal anode material for both K- and Ca-ion batteries with high performance. Journal of Power Sources, 2020, 480, 228876.	4.0	28
36	Self-consistent determination of Hubbard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math>for explaining the anomalous magnetism of the Gd<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>13</mml:mn></mml:msub></mml:math>cluster. Physical Review B, 2014, 89, .	1.1	26

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37	Edge-State-Enhanced CO₂ Electroreduction on Topological Nodal-Line Semimetal Cu₂Si Nanoribbons. Journal of Physical Chemistry C, 2019, 123, 2837-2842.	1.5	26
38	A new porous metallic silicon dicarbide for highly efficient Li-ion battery anode identified by targeted structure search. Carbon, 2018, 140, 680-687.	5.4	25
39	Assembling Si₂BN nanoribbons into a 3D porous structure as a universal anode material for both Li- and Na-ion batteries with high performance. Nanoscale, 2020, 12, 19367-19374.	2.8	25
40	Graphdiyneâ€Based Monolayers as Promising Anchoring Materials for Lithiumâ€“Sulfur Batteries: A Theoretical Study. Advanced Theory and Simulations, 2020, 3, 1900236.	1.3	21
41	Interpenetrating silicene networks: A topological nodal-line semimetal with potential as an anode material for sodium ion batteries. Physical Review Materials, 2018, 2, .	0.9	21
42	Borophene-Based Three-Dimensional Porous Structures as Anode Materials for Alkali Metal-Ion Batteries with Ultrahigh Capacity. Chemistry of Materials, 2021, 33, 2976-2983.	3.2	20
43	A stable metallic 3D porous BPC₂ as a universal anode material for Li, Na, and K ion batteries with high performance. Journal of Materials Chemistry A, 2020, 8, 25824-25830.	5.2	18
44	Recent advances in topological quantum anode materials for metal-ion batteries. Journal of Power Sources, 2022, 540, 231655.	4.0	18
45	New allotropes of Li₂MnO₃ as cathode materials with better cycling performance predicted in high pressure synthesis. Journal of Materials Chemistry A, 2017, 5, 16936-16943.	5.2	17
46	B₄ Cluster-Based 3D Porous Topological Metal as an Anode Material for Both Li- and Na-Ion Batteries with a Superhigh Capacity. Journal of Physical Chemistry Letters, 2021, 12, 1548-1553.	2.1	16
47	Three dimensional metallic porous SiC4 allotropes: Stability and battery applications. Nano Energy, 2019, 63, 103862.	8.2	15
48	Mechanisms of Ionic Diffusion and Stability of the Na₄MnCr(PO₄)₃ Cathode. , 2022, 4, 860-867.		13
49	A BN analog of two-dimensional triphenylene-graphdiyne: stability and properties. Nanoscale, 2019, 11, 9000-9007.	2.8	12
50	Screening Topological Quantum Materials for Na-Ion Battery Cathode. , 2022, 4, 175-180.		12
51	Tuning the Properties of Tetraceneâ€Based Nanoribbons by Fluorination and Nâ€Doping. ChemPhysChem, 2019, 20, 2799-2805.	1.0	10
52	Discovery of a high-pressure phase of rutile-like CoO₂ and its potential as a cathode material. Journal of Materials Chemistry A, 2018, 6, 18449-18457.	5.2	9
53	A topological semimetal Li₂CrN₂ sheet as a promising hydrogen storage material. Nanoscale, 2020, 12, 12106-12113.	2.8	9
54	Geometry, Electronic Properties, and Hydrogen Adsorption Properties of Li₃N-Based Nanostructures. Journal of Physical Chemistry C, 2010, 114, 19202-19205.	1.5	8

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55	Assembling Ï€-Conjugated Molecules with Negative Gaussian Curvature for Efficient Carbon-Based Metal-Free Thermoelectric Material. Journal of Physical Chemistry C, 2016, 120, 27829-27833.	1.5	7
56	Design of Three-Dimensional Metallic Biphenylene Networks for Na-Ion Battery Anodes with a Record High Capacity. ACS Applied Materials & Interfaces, 2022, 14, 32043-32055.	4.0	7
57	Dependence of Magnetism on Doping Concentration in V-Doped Bulk ZnO. Materials Transactions, 2008, 49, 2469-2473.	0.4	6
58	Tripyrrylmethane based 2D porous structure for hydrogen storage. Frontiers of Physics, 2011, 6, 220-223.	2.4	6
59	A high-pressure induced stable phase of Li₂MnSiO₄ as an effective poly-anion cathode material from simulations. Journal of Materials Chemistry A, 2019, 7, 16406-16413.	5.2	6
60	Three-dimensional porous borocarbonitride BC₂N with negative Poisson's ratio. Journal of Materials Chemistry C, 2020, 8, 15771-15777.	2.7	5
61	Triphenylene and tetracene based porous sheet: Stability and electronic properties. Computational Materials Science, 2020, 176, 109529.	1.4	4
62	Topological Quantum Cathode Materials for Fast Charging Liâ€Ion Battery Identified by Machine Learning and First Principles Calculation. Advanced Theory and Simulations, 2022, 5, 2100350.	1.3	4
63	3D Porous Metallic Boron Carbide Crystal Structure with Excellent Ductility. Advanced Theory and Simulations, 2021, 4, 2100325.	1.3	3
64	COMPUTATIONAL DESIGN OF NANOMATERIALS FOR HYDROGEN STORAGE. , 2009, , .		2
65	Enhancing Electron Emission of Hf with an Ultralow Work Function by Bariumâ€“Oxygen Coatings. Journal of Physical Chemistry C, 2022, 126, 2806-2812.	1.5	2
66	Probing the existence of energetically degenerate cluster isomers by chemical tagging. Applied Physics Letters, 2010, 97, 223104.	1.5	1
67	A Stable Threeâ€Dimensional Porous Carbon as a Highâ€Performance Anode Material for Lithium, Sodium, and Potassium Ion Batteries. Advanced Theory and Simulations, 0, , 2200230.	1.3	1
68	Research in renewable energy materials: The fundamental physics and chemistry China. Frontiers of Physics, 2011, 6, 141-141.	2.4	0