Penghao Xiao

List of Publications by Year in descending order

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47	3,529	236833	243529
papers	citations	25 h-index	44 g-index

49	49	49	5982
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A generalized solid-state nudged elastic band method. Journal of Chemical Physics, 2012, 136, 074103.	1.2	701
2	Removal of Interstitial H₂O in Hexacyanometallates for a Superior Cathode of a Sodium-Ion Battery. Journal of the American Chemical Society, 2015, 137, 2658-2664.	6.6	654
3	Simple Synthesis of Nanocrystalline Tin Sulfide/N-Doped Reduced Graphene Oxide Composites as Lithium Ion Battery Anodes. ACS Nano, 2016, 10, 10778-10788.	7.3	178
4	Additional Sodium Insertion into Polyanionic Cathodes for Higherâ€Energy Naâ€Ion Batteries. Advanced Energy Materials, 2017, 7, 1700514.	10.2	157
5	Linear topology in amorphous metal oxide electrochromic networks obtained via low-temperature solution processing. Nature Materials, 2016, 15, 1267-1273.	13.3	155
6	Solid-state dimer method for calculating solid-solid phase transitions. Journal of Chemical Physics, 2014, 140, 174104.	1.2	112
7	Interfacial adhesion between graphene and silicon dioxide by density functional theory with van der Waals corrections. Journal Physics D: Applied Physics, 2014, 47, 255301.	1.3	109
8	Calculations of Oxygen Stability in Lithium-Rich Layered Cathodes. Journal of Physical Chemistry C, 2012, 116, 23201-23204.	1.5	104
9	A highly efficient double-hierarchical sulfur host for advanced lithiumâ€“sulfur batteries. Chemical Science, 2018, 9, 666-675.	3.7	97
10	Theoretical Study of the Structural Evolution of a Na₂FeMn(CN)₆ Cathode upon Na Intercalation. Chemistry of Materials, 2015, 27, 3763-3768.	3.2	94
11	Theoretical and Experimental Study of Vanadium-Based Fluorophosphate Cathodes for Rechargeable Batteries. Chemistry of Materials, 2014, 26, 3089-3097.	3.2	90
12	Morphological Dependence of Lithium Insertion in Nanocrystalline TiO₂(B) Nanoparticles and Nanosheets. Journal of Physical Chemistry Letters, 2012, 3, 2015-2019.	2.1	87
13	Breaking Down the Crystallinity: The Path for Advanced Lithium Batteries. Advanced Energy Materials, 2016, 6, 1501933.	10.2	77
14	Understanding Surface Densified Phases in Ni-Rich Layered Compounds. ACS Energy Letters, 2019, 4, 811-818.	8.8	64
15	Enhanced Charge-Transfer Kinetics by Anion Surface Modification of LiFePO₄. Chemistry of Materials, 2012, 24, 3212-3218.	3.2	62
16	Unification of algorithms for minimum mode optimization. Journal of Chemical Physics, 2014, 140, 044115.	1.2	62
17	Engineering the Mechanical Properties of Monolayer Graphene Oxide at the Atomic Level. Journal of Physical Chemistry Letters, 2016, 7, 2702-2707.	2.1	60
18	Sodium Intercalation Behavior of Layered Na_xNbS₂ (0 â‰ x â‰ 1). Chemistry of Materials, 2013, 25, 1699-1705.	3.2	58

#	Article	IF	Citations
19	Highly reversible oxygen redox in layered compounds enabled by surface polyanions. Nature Communications, 2020, 11, 3411.	5.8	54
20	Suppressing the bipolar contribution to the thermoelectric properties of Mg2Si0.4Sn0.6 by Ge substitution. Journal of Applied Physics, 2015, 117, .	1.1	51
21	Kinetic Monte Carlo Study of Li Intercalation in LiFePO₄. ACS Nano, 2018, 12, 844-851.	7.3	47
22	Benchmarks for Characterization of Minima, Transition States, and Pathways in Atomic, Molecular, and Condensed Matter Systems. Journal of Chemical Theory and Computation, 2014, 10, 5476-5482.	2.3	43
23	Investigation and Suppression of Oxygen Release by LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂ Cathode under Overcharge Conditions. Advanced Energy Materials, 2022, 12, .	10.2	40
24	In Situ Raman Study of Phase Stability of Î±-Li₃V₂(PO₄)₃ upon Thermal and Laser Heating. Journal of Physical Chemistry C, 2013, 117, 11994-12002.	1.5	39
25	Communication: From graphite to diamond: Reaction pathways of the phase transition. Journal of Chemical Physics, 2012, 137, 101101.	1.2	33
26	Simulation of Potential-Dependent Activation Energies in Electrocatalysis: Mechanism of Oâ€“O Bond Formation on RuO₂. Journal of Physical Chemistry C, 2021, 125, 15243-15250.	1.5	28
27	Calculations of oxide formation on low-index Cu surfaces. Journal of Chemical Physics, 2016, 145, 044711.	1.2	25
28	Wide electrochemical window ionic salt for use in electropositive metal electrodeposition and solid state Li-ion batteries. Journal of Materials Chemistry A, 2014, 2, 2194-2201.	5.2	23
29	Transformation of topologically close-packed Î²-W to body-centered cubic Î±-W: Comparison of experiments and computations. Journal of Chemical Physics, 2017, 147, 152709.	1.2	22
30	Fast Mg2+ diffusion in Mo3(PO4)3O for Mg batteries. Chemical Communications, 2017, 53, 7998-8001.	2.2	22
31	Structural transformations in Li₂MnSiO₄: evidence that a Li intercalation material can reversibly cycle through a disordered phase. Journal of Materials Chemistry A, 2017, 5, 16722-16731.	5.2	22
32	Effect of fluorination and Li-excess on the Li migration barrier in Mn-based cathode materials. Journal of Materials Chemistry A, 2020, 8, 19965-19974.	5.2	20
33	Shear-Assisted Formation of Cation-Disordered Rocksalt NaMO₂ (M = Fe or Mn). Chemistry of Materials, 2018, 30, 8811-8821.	3.2	17
34	Mechanism of the CaIrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>post-perovskite phase transition under pressure. Physical Review B, 2013, 88, .	1.1	16
35	Nudged elastic band method for solid-solid transition under finite deformation. Journal of Chemical Physics, 2019, 151, .	1.2	14
36	Spontaneous dynamical disordering of borophenes in MgB2 and related metal borides. Nature Communications, 2021, 12, 6268.	5.8	14

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37	Superior Oxygen Electrocatalysis on RuSe x Nanoparticles for Rechargeable Air Cathodes. Advanced Energy Materials, 2018, 8, 1702037.	10.2	13
38	Detonation-induced transformation of graphite to hexagonal diamond. Physical Review B, 2020, 102, .	1.1	13
39	Calculations of Oxygen Adsorption-Induced Surface Reconstruction and Oxide Formation on Cu(100). Chemistry of Materials, 2017, 29, 1472-1484.	3.2	12
40	Basin constrained Îº-dimer method for saddle point finding. Journal of Chemical Physics, 2014, 141, 164111.	1.2	10
41	Localized Mg-vacancy states in the thermoelectric material Mg2âˆ’Î´Si0.4Sn0.6. Journal of Applied Physics, 2016, 119, .	1.1	9
42	Communication: Calculations of the (2 Ã— 1)-O reconstruction kinetics on Cu(110). Journal of Chemical Physics, 2017, 146, 111101.	1.2	8
43	Ridge-based bias potentials to accelerate molecular dynamics. Journal of Chemical Physics, 2015, 143, 244104.	1.2	7
44	PTCDA Molecular Monolayer on Pb Thin Films: An Unusual <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math> -Electron Kondo System and Its Interplay with a Quantum-Confined Superconductor. Physical Review Letters, 2021, 127, 186805.	2.9	6
45	Oxide Scale Evolution on Binary Alloys: Transient State Kinetics from First Principles. ECS Meeting Abstracts, 2020, MA2020-02, 1176-1176.	0.0	0
46	The Asymmetric Charge-Discharge Kinetics in Li_{1-X}Ni_{1+X}O₂ from First Principles. ECS Meeting Abstracts, 2022, MA2022-01, 447-447.	0.0	0
47	Atomic-Scale Oxide Growth and Dissolution Kinetics on Ni-Cr Alloys. ECS Meeting Abstracts, 2022, MA2022-01, 1006-1006.	0.0	0