

Penghao Xiao

List of Publications by Year in descending order

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47
papers

3,529
citations

236833

25
h-index

243529

44
g-index

49
all docs

49
docs citations

49
times ranked

5982
citing authors

#	ARTICLE	IF	CITATIONS
1	Investigation and Suppression of Oxygen Release by $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ Cathode under Overcharge Conditions. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	40
2	The Asymmetric Charge-Discharge Kinetics in $\text{Li}_{1-x}\text{Ni}_{1+x}\text{O}_2$ from First Principles. <i>ECS Meeting Abstracts</i> , 2022, MA2022-01, 447-447.	0.0	0
3	Atomic-Scale Oxide Growth and Dissolution Kinetics on Ni-Cr Alloys. <i>ECS Meeting Abstracts</i> , 2022, MA2022-01, 1006-1006.	0.0	0
4	Simulation of Potential-Dependent Activation Energies in Electrocatalysis: Mechanism of O-O Bond Formation on RuO_2 . <i>Journal of Physical Chemistry C</i> , 2021, 125, 15243-15250.	1.5	28
5	PTCDA Molecular Monolayer on Pb Thin Films: An Unusual π -Electron Kondo System and Its Interplay with a Quantum-Confined Superconductor. <i>Physical Review Letters</i> , 2021, 127, 186805.	2.9	6
6	Spontaneous dynamical disordering of borophenes in MgB_2 and related metal borides. <i>Nature Communications</i> , 2021, 12, 6268.	5.8	14
7	Effect of fluorination and Li-excess on the Li migration barrier in Mn-based cathode materials. <i>Journal of Materials Chemistry A</i> , 2020, 8, 19965-19974.	5.2	20
8	Detonation-induced transformation of graphite to hexagonal diamond. <i>Physical Review B</i> , 2020, 102, .	1.1	13
9	Highly reversible oxygen redox in layered compounds enabled by surface polyanions. <i>Nature Communications</i> , 2020, 11, 3411.	5.8	54
10	Oxide Scale Evolution on Binary Alloys: Transient State Kinetics from First Principles. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 1176-1176.	0.0	0
11	Nudged elastic band method for solid-solid transition under finite deformation. <i>Journal of Chemical Physics</i> , 2019, 151, .	1.2	14
12	Understanding Surface Densified Phases in Ni-Rich Layered Compounds. <i>ACS Energy Letters</i> , 2019, 4, 811-818.	8.8	64
13	Kinetic Monte Carlo Study of Li Intercalation in LiFePO_4 . <i>ACS Nano</i> , 2018, 12, 844-851.	7.3	47
14	Superior Oxygen Electrocatalysis on RuSe_x Nanoparticles for Rechargeable Air Cathodes. <i>Advanced Energy Materials</i> , 2018, 8, 1702037.	10.2	13
15	A highly efficient double-hierarchical sulfur host for advanced lithium-sulfur batteries. <i>Chemical Science</i> , 2018, 9, 666-675.	3.7	97
16	Shear-Assisted Formation of Cation-Disordered Rocksalt NaMO_2 (M = Fe or Mn). <i>Chemistry of Materials</i> , 2018, 30, 8811-8821.	3.2	17
17	Calculations of Oxygen Adsorption-Induced Surface Reconstruction and Oxide Formation on $\text{Cu}(100)$. <i>Chemistry of Materials</i> , 2017, 29, 1472-1484.	3.2	12
18	Additional Sodium Insertion into Polyanionic Cathodes for Higher-Energy Na-Ion Batteries. <i>Advanced Energy Materials</i> , 2017, 7, 1700514.	10.2	157

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19	Communication: Calculations of the (2 Å ⁻¹) ₀ reconstruction kinetics on Cu(110). Journal of Chemical Physics, 2017, 146, 111101.	1.2	8
20	Transformation of topologically close-packed \hat{I}^2 -W to body-centered cubic \hat{I}^{\pm} -W: Comparison of experiments and computations. Journal of Chemical Physics, 2017, 147, 152709.	1.2	22
21	Fast Mg ²⁺ diffusion in Mo ₃ (PO ₄) ₃ O for Mg batteries. Chemical Communications, 2017, 53, 7998-8001.	2.2	22
22	Structural transformations in Li ₂ MnSiO ₄ : 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
23	Breaking Down the Crystallinity: The Path for Advanced Lithium Batteries. Advanced Energy Materials, 2016, 6, 1501933.	10.2	77
24	Calculations of oxide formation on low-index Cu surfaces. Journal of Chemical Physics, 2016, 145, 044711.	1.2	25
25	Localized Mg-vacancy states in the thermoelectric material Mg ₂ Si _{0.4} Sn _{0.6} . Journal of Applied Physics, 2016, 119, .	1.1	9
26	Linear topology in amorphous metal oxide electrochromic networks obtained via low-temperature solution processing. Nature Materials, 2016, 15, 1267-1273.	13.3	155
27	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
28	Engineering the Mechanical Properties of Monolayer Graphene Oxide at the Atomic Level. Journal of Physical Chemistry Letters, 2016, 7, 2702-2707.	2.1	60
29	Ridge-based bias potentials to accelerate molecular dynamics. Journal of Chemical Physics, 2015, 143, 244104.	1.2	7
30	Suppressing the bipolar contribution to the thermoelectric properties of Mg ₂ Si _{0.4} Sn _{0.6} by Ge substitution. Journal of Applied Physics, 2015, 117, .	1.1	51
31	Removal of Interstitial H ₂ O in Hexacyanometallates for a Superior Cathode of a Sodium-Ion Battery. Journal of the American Chemical Society, 2015, 137, 2658-2664.	6.6	654
32	Theoretical Study of the Structural Evolution of a Na ₂ FeMn(CN) ₆ Cathode upon Na Intercalation. Chemistry of Materials, 2015, 27, 3763-3768.	3.2	94
33	Unification of algorithms for minimum mode optimization. Journal of Chemical Physics, 2014, 140, 044115.	1.2	62
34	Basin constrained \hat{I}^{\pm} -dimer method for saddle point finding. Journal of Chemical Physics, 2014, 141, 164111.	1.2	10
35	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
36	Solid-state dimer method for calculating solid-solid phase transitions. Journal of Chemical Physics, 2014, 140, 174104.	1.2	112

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37	Benchmarks for Characterization of Minima, Transition States, and Pathways in Atomic, Molecular, and Condensed Matter Systems. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5476-5482.	2.3	43
38	Theoretical and Experimental Study of Vanadium-Based Fluorophosphate Cathodes for Rechargeable Batteries. <i>Chemistry of Materials</i> , 2014, 26, 3089-3097.	3.2	90
39	Interfacial adhesion between graphene and silicon dioxide by density functional theory with van der Waals corrections. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 255301.	1.3	109
40	Sodium Intercalation Behavior of Layered NaNb_2O_7 (0 \times 1). <i>Chemistry of Materials</i> , 2013, 25, 1699-1705.	3.2	58
41	Mechanism of the CaIrO_3 post-perovskite phase transition under pressure. <i>Physical Review B</i> , 2013, 88, .	1.1	16
42	In Situ Raman Study of Phase Stability of $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ upon Thermal and Laser Heating. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11994-12002.	1.5	39
43	A generalized solid-state nudged elastic band method. <i>Journal of Chemical Physics</i> , 2012, 136, 074103.	1.2	701
44	Communication: From graphite to diamond: Reaction pathways of the phase transition. <i>Journal of Chemical Physics</i> , 2012, 137, 101101.	1.2	33
45	Morphological Dependence of Lithium Insertion in Nanocrystalline $\text{TiO}_2(\text{B})$ Nanoparticles and Nanosheets. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2015-2019.	2.1	87
46	Enhanced Charge-Transfer Kinetics by Anion Surface Modification of LiFePO_4 . <i>Chemistry of Materials</i> , 2012, 24, 3212-3218.	3.2	62
47	Calculations of Oxygen Stability in Lithium-Rich Layered Cathodes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23201-23204.	1.5	104