

Houlong L Zhuang

List of Publications by Year in descending order

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64
papers

5,476
citations

147801

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118850

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all docs

67
docs citations

67
times ranked

8133
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational Screening of 2D Materials for Photocatalysis. Journal of Physical Chemistry Letters, 2015, 6, 1087-1098.	4.6	641
2	Ab Initio Prediction of Piezoelectricity in Two-Dimensional Materials. ACS Nano, 2015, 9, 9885-9891.	14.6	445
3	Strong anisotropy and magnetostriction in the two-dimensional Stoner ferromagnet Fe_2P . Physical Review B, 2016, 93, .	8.2	299
4	Machine-learning phase prediction of high-entropy alloys. Acta Materialia, 2019, 169, 225-236.	7.9	297
5	Enhanced Li-S Batteries Using Amine-Functionalized Carbon Nanotubes in the Cathode. ACS Nano, 2016, 10, 1050-1059.	14.6	289
6	Electrochemical surface passivation of LiCoO ₂ particles at ultrahigh voltage and its applications in lithium-based batteries. Nature Communications, 2018, 9, 4918.	12.8	260
7	Regulating Li deposition at artificial solid electrolyte interphases. Journal of Materials Chemistry A, 2017, 5, 3483-3492.	10.3	258
8	A cation-anion regulation synergistic anode host for dendrite-free lithium metal batteries. Science Advances, 2018, 4, eaar4410.	10.3	241
9	Accuracy of exchange-correlation functionals and effect of solvation on the surface energy of copper. Physical Review B, 2013, 87, .	3.2	211
10	Stable Lithium Electrodeposition at Ultra-High Current Densities Enabled by 3D PMF/Li Composite Anode. Advanced Energy Materials, 2018, 8, 1703360.	19.5	194
11	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	8.7	181
12	Stability and magnetism of strongly correlated single-layer VS_2 . Physical Review B, 2016, 93, .	8.2	176
13	Machine learning for phase selection in multi-principal element alloys. Computational Materials Science, 2018, 150, 230-235.	3.0	174
14	Enabling Stable Lithium Metal Anode via 3D Inorganic Skeleton with Superlithiophilic Interphase. Advanced Energy Materials, 2018, 8, 1802350.	19.5	147
15	Room-Temperature Synthesis of 2D Janus Crystals and their Heterostructures. Advanced Materials, 2020, 32, e2006320.	21.0	138
16	Ultrahigh-Rate and Long-Life Zinc-Metal Anodes Enabled by Self-Accelerated Cation Migration. Advanced Energy Materials, 2021, 11, 2100982.	19.5	131
17	Hybrid cathode architectures for lithium batteries based on TiS_2 and sulfur. Journal of Materials Chemistry A, 2015, 3, 19857-19866.	10.3	119
18	Electronic structures of single-layer boron pnictides. Applied Physics Letters, 2012, 101, .	3.3	114

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19	A Density Functional Assessment of Oxygen Evolution Reaction Mechanisms on \hat{P}^2 -NiOOH. ACS Catalysis, 2017, 7, 5329-5339.	11.2	110
20	Computational prediction and characterization of single-layer CrS ₂ . Applied Physics Letters, 2014, 104, 022116.	3.3	108
21	Surface Energy as a Descriptor of Catalytic Activity. Journal of Physical Chemistry C, 2016, 120, 23698-23706.	3.1	83
22	Tethered Molecular Sorbents: Enabling Metal-Sulfur Battery Cathodes. Advanced Energy Materials, 2014, 4, 1400390.	19.5	67
23	Doping-controlled phase transitions in single-layer MoS_2 . Physical Review B, 2017, 96, .		
24	Computational identification of single-layer CdO for electronic and optical applications. Applied Physics Letters, 2013, 103, .	3.3	52
25	Density functional theory study of bulk and single-layer magnetic semiconductor CrPS_4 . Physical Review B, 2016, 94, .		
26	A percolation theory for designing corrosion-resistant alloys. Nature Materials, 2021, 20, 789-793.	27.5	48
27	Computational Discovery, Characterization, and Design of Single-Layer Materials. Jom, 2014, 66, 366-374.	1.9	41
28	Petascale Orbital-Free Density Functional Theory Enabled by Small-Box Algorithms. Journal of Chemical Theory and Computation, 2016, 12, 2950-2963.	5.3	41
29	Anomalous Behavior of 2D Janus Excitonic Layers under Extreme Pressures. Advanced Materials, 2020, 32, e2002401.	21.0	36
30	Disordered hyperuniformity in two-dimensional amorphous silica. Science Advances, 2020, 6, eaba0826.	10.3	35
31	Can an element form a two-dimensional nanosheet of type 15 pentagons?. Computational Materials Science, 2018, 154, 37-40.	3.0	34
32	Interface orbital engineering of large-gap topological states: Decorating gold on a Si(111) surface. Physical Review B, 2016, 93, .	3.2	32
33	Elastic and Thermodynamic Properties of Complex Mg-Al Intermetallic Compounds via Orbital-Free Density Functional Theory. Physical Review Applied, 2016, 5, .	3.8	30
34	Ultimate Control over Hydrogen Bond Formation and Reaction Rates for Scalable Synthesis of Highly Crystalline vdW MOF Nanosheets with Large Aspect Ratio. Advanced Materials, 2018, 30, e1802497.	21.0	30
35	Single-layer antiferromagnetic semiconductor CoS_2 with pentagonal structure. Physical Review B, 2018, 98, .		
36	Stone-Wales defects preserve hyperuniformity in amorphous two-dimensional networks. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	28

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37	Synthesis and Fundamental Studies of Si-Compatible (Si)GeSn and GeSn Mid-IR Systems with Ultrahigh Sn Contents. <i>Chemistry of Materials</i> , 2019, 31, 9831-9842.	6.7	26
38	Synthesis of a Smart Hybrid MXene with Switchable Conductivity for Temperature Sensing. <i>ACS Applied Nano Materials</i> , 2020, 3, 4069-4076.	5.0	26
39	From pentagonal geometries to two-dimensional materials. <i>Computational Materials Science</i> , 2019, 159, 448-453.	3.0	24
40	Abnormal band bowing effects in phase instability crossover region of GaSe _{1-x} Te _x nanomaterials. <i>Nature Communications</i> , 2018, 9, 1927.	12.8	20
41	Phase Transition across Anisotropic NbS ₃ and Direct Gap Semiconductor TiS ₃ at Nominal Titanium Alloying Limit. <i>Advanced Materials</i> , 2020, 32, 2000018.	21.0	16
42	Single-layer ferromagnetic and piezoelectric CoAsS with pentagonal structure. <i>APL Materials</i> , 2019, 7, .	5.1	14
43	$\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{PtP} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle$: An example of exploring the hidden Cairo tessellation in the pyrite structure for discovering novel two-dimensional materials. <i>Physical Review Materials</i> , 2018, 2, .	2.4	14
44	Electrical and thermal transport properties of medium-entropy Si Ge Sn alloys. <i>Acta Materialia</i> , 2020, 199, 443-452.	7.9	13
45	Semiconducting SiGeSn high-entropy alloy: A density functional theory study. <i>Journal of Applied Physics</i> , 2019, 126, 225703.	2.5	12
46	Nearly hyperuniform, nonhyperuniform, and antihyperuniform density fluctuations in two-dimensional transition metal dichalcogenides with defects. <i>Physical Review B</i> , 2021, 103, .	3.2	12
47	High-throughput Computational Characterization of 2D Compositionally Complex Transition-Metal Chalcogenide Alloys. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000195.	2.8	11
48	Computational prediction and characterization of two-dimensional pentagonal arsenopyrite FeAsS. <i>Computational Materials Science</i> , 2019, 166, 105-110.	3.0	9
49	<i>Ab initio</i> playing of pentagonal puzzles. <i>Electronic Structure</i> , 2019, 1, 015004.	2.8	7
50	Topological transformations in hyperuniform pentagonal two-dimensional materials induced by Stone-Wales defects. <i>Physical Review B</i> , 2021, 103, .	3.2	7
51	Sudoku-inspired high-Shannon-entropy alloys. <i>Acta Materialia</i> , 2022, 225, 117556.	7.9	5
52	Toward obtaining 2D and 3D and 1D PtPN with pentagonal pattern. <i>Journal of Materials Science</i> , 2019, 54, 14029-14037.	3.7	4
53	Dimension engineering of single-layer PtN ₂ with the Cairo tessellation. <i>Journal of Applied Physics</i> , 2019, 125, 204302.	2.5	4
54	From evidence to new high-entropy alloys. <i>Nature Computational Science</i> , 2021, 1, 458-459.	8.0	4

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55	Scalable nanomanufacturing of holey graphene <i>via</i> chemical etching: an investigation into process mechanisms. <i>Nanoscale</i> , 2022, 14, 4762-4769.	5.6	4
56	Orbital-free density functional theory characterization of the Mg_2Al phase. <i>Physical Review B</i> , 2021, 103, 040401.	2.4	3
57	High-throughput functionalization of single-layer electride Ca ₂ N. <i>Materials Research Express</i> , 2018, 5, 076306.	1.6	2
58	Synthesis of heteroepitaxial BP and related Al-B-Sb-As-P films via CVD of Al(BH ₄) ₃ and MH ₃ (M=P, As, Sb) at temperatures below 600 Å°C. <i>Semiconductor Science and Technology</i> , 2020, 35, 085034.	2.0	2
59	Spin qubit based on the nitrogen-vacancy center analog in a diamond-like compound C ₃ BN. <i>Journal of Applied Physics</i> , 2021, 130, .	2.5	2
60	First-Principles Study on the 1T Phase of GaX (X=S, Se) Monolayers. <i>ChemistrySelect</i> , 2016, 1, 5779-5783.	1.5	1
61	Quantum Materials for Energy-Efficient Computing. <i>Jom</i> , 2020, 72, 3147-3148.	1.9	0
62	A Tribute to Emily A. Carter. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1669-1670.	2.5	0
63	A Tribute to Emily A. Carter. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4331-4332.	3.1	0
64	Understanding the mechanism of shockwave induced graphite-to-diamond phase transition. <i>Materialia</i> , 2022, 24, 101487.	2.7	0