Peilin Liao

List of Publications by Year in descending order

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45 papers	4,856 citations	218677 26 h-index	233421 45 g-index
47 all docs	47 docs citations	47 times ranked	7282 citing authors

#	Article	IF	Citations
1	Layer-by-layer anionic diffusion in two-dimensional halide perovskite vertical heterostructures. Nature Nanotechnology, 2021, 16, 584-591.	31.5	88
2	Doping-Enabled Reconfigurable Strongly Correlated Phase in a Quasi-2D Perovskite. Journal of Physical Chemistry Letters, 2021, 12, 5091-5098.	4.6	1
3	Catalytic Light Alkanes Conversion through Anaerobic Ammodehydrogenation. ACS Catalysis, 2021, 11, 7987-7995.	11.2	8
4	Ligand-Driven Grain Engineering of High Mobility Two-Dimensional Perovskite Thin-Film Transistors. Journal of the American Chemical Society, 2021, 143, 15215-15223.	13.7	55
5	Neural network reactive force field for C, H, N, and O systems. Npj Computational Materials, 2021, 7, .	8.7	39
6	Facile Synthesis of Pt Carbide Nanomaterials and Their Catalytic Applications. , 2021, 3, 179-186.		8
7	Parallel Nanoimprint Forming of One-Dimensional Chiral Semiconductor for Strain-Engineered Optical Properties. Nano-Micro Letters, 2020, 12, 160.	27.0	8
8	Strainâ€Engineered Anisotropic Optical and Electrical Properties in 2D Chiralâ€Chain Tellurium. Advanced Materials, 2020, 32, e2002342.	21.0	40
9	First principles study on hydrogen doping induced metal-to-insulator transition in rare earth nickelates RNiO₃ (R = Pr, Nd, Sm, Eu, Gd, Tb, Dy, Yb). Physical Chemistry Chemical Physics, 2020, 22, 6888-6895.	2.8	23
10	A Surfaceâ€Oxideâ€Rich Activation Layer (SOAL) on Ni₂Mo₃N for a Rapid and Durable Oxygen Evolution Reaction. Angewandte Chemie - International Edition, 2020, 59, 18036-18041.	13.8	77
11	A Surfaceâ€Oxideâ€Rich Activation Layer (SOAL) on Ni 2 Mo 3 N for a Rapid and Durable Oxygen Evolution Reaction. Angewandte Chemie, 2020, 132, 18192-18197.	2.0	4
12	Structural Tunability and Diversity of Twoâ€Dimensional Lead Halide Benzenethiolate. Chemistry - A European Journal, 2020, 26, 6599-6607.	3.3	3
13	Online simulation powered learning modules for materials science. MRS Advances, 2019, 4, 2727-2742.	0.9	1
14	Chiral features of metal phthalocyanines sitting atop the pre-assembled TiOPc monolayer on Ag(111). Physical Chemistry Chemical Physics, 2019, 21, 16323-16328.	2.8	5
15	Distribution and Valence State of Ru Species on CeO₂ Supports: Support Shape Effect and Its Influence on CO Oxidation. ACS Catalysis, 2019, 9, 11088-11103.	11.2	159
16	Molecular engineering of organicâ€“inorganic hybrid perovskites quantum wells. Nature Chemistry, 2019, 11, 1151-1157.	13.6	302
17	Highly Stable Lead-Free Perovskite Field-Effect Transistors Incorporating Linear Ï€-Conjugated Organic Ligands. Journal of the American Chemical Society, 2019, 141, 15577-15585.	13.7	180
18	Interfacial Sites between Cobalt Nitride and Cobalt Act as Bifunctional Catalysts for Hydrogen Electrochemistry. ACS Energy Letters, 2019, 4, 1594-1601.	17.4	128

#	Article	IF	Citations
19	Steering the Achiral into Chiral with a Self-Assembly Strategy. ACS Nano, 2019, 13, 7202-7208.	14.6	16
20	A computational study of hydrogen doping induced metal-to-insulator transition in CaFeO₃, SrFeO₃, BaFeO₃ and SmMnO₃. Physical Chemistry Chemical Physics, 2019, 21, 25397-25405.	2.8	8
21	Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. Catalysis Today, 2018, 312, 149-157.	4.4	16
22	Detection and Manipulation of Charge States for Double-Decker DyPc₂ Molecules on Ultrathin CuO Films. ACS Nano, 2018, 12, 2991-2997.	14.6	16
23	Metal-to-insulator transition in SmNiO₃ induced by chemical doping: a first principles study. Molecular Systems Design and Engineering, 2018, 3, 264-274.	3.4	24
24	Molecular Building Block-Based Electronic Charges for High-Throughput Screening of Metalâ€“Organic Frameworks for Adsorption Applications. Journal of Chemical Theory and Computation, 2018, 14, 365-376.	5.3	18
25	Interfacing nickel nitride and nickel boosts both electrocatalytic hydrogen evolution and oxidation reactions. Nature Communications, 2018, 9, 4531.	12.8	410
26	Insights into Catalytic Hydrolysis of Organophosphate Warfare Agents by Metalâ€“Organic Framework NU-1000. Journal of Physical Chemistry C, 2018, 122, 12362-12368.	3.1	55
27	Optimizing Open Iron Sites in Metalâ€“Organic Frameworks for Ethane Oxidation: A First-Principles Study. ACS Applied Materials & Interfaces, 2017, 9, 33484-33492.	8.0	44
28	Steering Onâ€Surface Reactions by a Selfâ€Assembly Approach. Angewandte Chemie - International Edition, 2017, 56, 5026-5030.	13.8	28
29	Steering Onâ€Surface Reactions by a Selfâ€Assembly Approach. Angewandte Chemie, 2017, 129, 5108-5112.	2.0	14
30	Alkaline-earth metal-oxide overlayers on TiO₂: application toward CO₂ photoreduction. Catalysis Science and Technology, 2016, 6, 7885-7895.	4.1	29
31	Stabilizing surface Ag adatoms into tunable single atom arrays by terminal alkyne assembly. Chemical Communications, 2016, 52, 12944-12947.	4.1	15
32	Destruction of chemical warfare agents using metalâ€“organic frameworks. Nature Materials, 2015, 14, 512-516.	27.5	790
33	Low-temperature scanning tunneling microscopy study on the electronic properties of a double-decker DyPc2 molecule at the surface. Physical Chemistry Chemical Physics, 2015, 17, 27019-27026.	2.8	22
34	Titanium incorporation into hematite photoelectrodes: theoretical considerations and experimental observations. Energy and Environmental Science, 2014, 7, 3100-3121.	30.8	118
35	New concepts and modeling strategies to design and evaluate photo-electro-catalysts based on transition metal oxides. Chemical Society Reviews, 2013, 42, 2401-2422.	38.1	225
36	Origin of the Energy Barrier to Chemical Reactions of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>on Al(111): Evidence for Charge Transfer, Not Spin Selection. Physical Review Letters, 2012, 109, 198303.	7.8	125

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37	Hole transport in pure and doped hematite. Journal of Applied Physics, 2012, 112, .	2.5	84
38	Water Oxidation on Pure and Doped Hematite (0001) Surfaces: Prediction of Co and Ni as Effective Dopants for Electrocatalysis. Journal of the American Chemical Society, 2012, 134, 13296-13309.	13.7	492
39	Testing variations of the GW approximation on strongly correlated transition metal oxides: hematite (Î±-Fe2O3) as a benchmark. Physical Chemistry Chemical Physics, 2011, 13, 15189.	2.8	135
40	Electron Transport in Pure and Doped Hematite. Nano Letters, 2011, 11, 1775-1781.	9.1	267
41	Optical Excitations in Hematite (Î±-Fe₂O₃) via Embedded Cluster Models: A CASPT2 Study. Journal of Physical Chemistry C, 2011, 115, 20795-20805.	3.1	57
42	First principles scheme to evaluate band edge positions in potential transition metal oxide photocatalysts and photoelectrodes. Physical Chemistry Chemical Physics, 2011, 13, 16644.	2.8	380
43	Ab initio density functional theory+U predictions of the shear response of iron oxides. Acta Materialia, 2010, 58, 5912-5925.	7.9	11
44	Ab initio DFT + U predictions of tensile properties of iron oxides. Journal of Materials Chemistry, 2010, 20, 6703.	6.7	45
45	Rotationally invariant ab initio evaluation of Coulomb and exchange parameters for DFT+U calculations. Journal of Chemical Physics, 2008, 129, 014103.	3.0	282