Gang Lu

List of Publications by Year
in descending order

98 papers	9,860 citations	71061 41 h-index	36008 97 g-index
99 all docs	99 docs citations	99 times ranked	11040 citing authors

#	Article	IF	Citations
1	Biaxially strained PtPb/Pt core/shell nanoplate boosts oxygen reduction catalysis. Science, 2016, 354, 1410-1414.	6.0	1,262
2	PdMo bimetallene for oxygen reduction catalysis. Nature, 2019, 574, 81-85.	13.7	935
3	Precise tuning in platinum-nickel/nickel sulfide interface nanowires for synergistic hydrogen evolution catalysis. Nature Communications, 2017, 8, 14580.	5.8	648
4	Surface engineering of hierarchical platinum-cobalt nanowires for efficient electrocatalysis. Nature Communications, 2016, 7, 11850.	5.8	607
5	Tuning Sn-Catalysis for Electrochemical Reduction of CO₂ to CO via the Core/Shell Cu/SnO₂ Structure. Journal of the American Chemical Society, 2017, 139, 4290-4293.	6.6	553
6	Efficient oxygen reduction catalysis by subnanometer Pt alloy nanowires. Science Advances, 2017, 3, e1601705.	4.7	330
7	Stable Highâ€Index Faceted Pt Skin on Zigzagâ€Like PtFe Nanowires Enhances Oxygen Reduction Catalysis. Advanced Materials, 2018, 30, 1705515.	11.1	305
8	A General Method for Multimetallic Platinum Alloy Nanowires as Highly Active and Stable Oxygen Reduction Catalysts. Advanced Materials, 2015, 27, 7204-7212.	11.1	280
9	Ordered PdCuâ€Based Nanoparticles as Bifunctional Oxygenâ€Reduction and Ethanolâ€Oxidation Electrocatalysts. Angewandte Chemie - International Edition, 2016, 55, 9030-9035.	7.2	278
10	A New Core/Shell NiAu/Au Nanoparticle Catalyst with Pt-like Activity for Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2015, 137, 5859-5862.	6.6	274
11	Hydrogen Embrittlement of Aluminum: The Crucial Role of Vacancies. Physical Review Letters, 2005, 94, 155501.	2.9	234
12	Surface Doping to Enhance Structural Integrity and Performance of Liâ€Rich Layered Oxide. Advanced Energy Materials, 2018, 8, 1802105.	10.2	228
13	Steering elementary steps towards efficient alkaline hydrogen evolution via size-dependent Ni/NiO nanoscale heterosurfaces. National Science Review, 2020, 7, 27-36.	4.6	192
14	Cu₃N Nanocubes for Selective Electrochemical Reduction of CO₂ to Ethylene. Nano Letters, 2019, 19, 8658-8663.	4.5	173
15	Core/Shell Face-Centered Tetragonal FePd/Pd Nanoparticles as an Efficient Non-Pt Catalyst for the Oxygen Reduction Reaction. ACS Nano, 2015, 9, 11014-11022.	7.3	165
16	Exclusive Strain Effect Boosts Overall Water Splitting in PdCu/Ir Core/Shell Nanocrystals. Angewandte Chemie - International Edition, 2021, 60, 8243-8250.	7.2	163
17	Tungstenâ€Doped L1₀â€PtCo Ultrasmall Nanoparticles as a Highâ€Performance Fuel Cell Cathode. Angewandte Chemie - International Edition, 2019, 58, 15471-15477.	7.2	150
18	Hydrogen-Enhanced Local Plasticity in Aluminum: AnAb InitioStudy. Physical Review Letters, 2001, 87, 095501.	2.9	135

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19	Interfacial Oxygen Vacancies as a Potential Cause of Hysteresis in Perovskite Solar Cells. Chemistry of Materials, 2016, 28, 802-812.	3.2	128
20	Subâ€6 nm Fully Ordered L1₀â€Ptâ€“Niâ€“Co Nanoparticles Enhance Oxygen Reduction via Co Doping Induced Ferromagnetism Enhancement and Optimized Surface Strain. Advanced Energy Materials, 2019, 9, 1803771.	10.2	127
21	Biaxial Strains Mediated Oxygen Reduction Electrocatalysis on Fenton Reaction Resistant L1₀â€PtZn Fuel Cell Cathode. Advanced Energy Materials, 2020, 10, 2000179.	10.2	112
22	Iron migration and oxygen oxidation during sodium extraction from NaFeO2. Nano Energy, 2018, 47, 519-526.	8.2	111
23	Ultrathin PtPdâ€Based Nanorings with Abundant Step Atoms Enhance Oxygen Catalysis. Advanced Materials, 2018, 30, e1802136.	11.1	107
24	Bifunctional Atomically Dispersed Moâ€“N₂/C Nanosheets Boost Lithium Sulfide Deposition/Decomposition for Stable Lithiumâ€“Sulfur Batteries. ACS Nano, 2020, 14, 10115-10126.	7.3	106
25	From electrons to finite elements: A concurrent multiscale approach for metals. Physical Review B, 2006, 73, .	1.1	103
26	Improving the Stability of Nonâ€Nobleâ€Metal Mâ€“Nâ€“C Catalysts for Protonâ€Exchangeâ€Membrane Fuel Cells through Mâ€“N Bond Length and Coordination Regulation. Advanced Materials, 2021, 33, e2006613.	11.1	94
27	How Methylammonium Cations and Chlorine Dopants Heal Defects in Lead Iodide Perovskites. Advanced Energy Materials, 2018, 8, 1702754.	10.2	86
28	Subâ€Monolayer YO_x/MoO_x on Ultrathin Pt Nanowires Boosts Alcohol Oxidation Electrocatalysis. Advanced Materials, 2021, 33, e2103762.	11.1	86
29	Understanding Ultrafast Rechargeable Aluminum-Ion Battery from First-Principles. Journal of Physical Chemistry C, 2017, 121, 7131-7138.	1.5	84
30	Computational Screening of Near-Surface Alloys for CO₂ Electroreduction. ACS Catalysis, 2018, 8, 3885-3894.	5.5	79
31	Lavender-Like Ga-Doped Pt₃Co Nanowires for Highly Stable and Active Electrocatalysis. ACS Catalysis, 2020, 10, 3018-3026.	5.5	75
32	Anti-dissolution Pt single site with Pt(OH)(O3)/Co(P) coordination for efficient alkaline water splitting electrolyzer. Nature Communications, 2022, 13, .	5.8	73
33	Computational Design of Core/Shell Nanoparticles for Oxygen Reduction Reactions. Journal of Physical Chemistry Letters, 2014, 5, 292-297.	2.1	71
34	Native Vacancy Enhanced Oxygen Redox Reversibility and Structural Robustness. Advanced Energy Materials, 2019, 9, 1803087.	10.2	70
35	Cu-Based Single-Atom Catalysts Boost Electroreduction of CO₂ to CH₃OH: First-Principles Predictions. Journal of Physical Chemistry C, 2019, 123, 4380-4387.	1.5	68
36	Overpotential for CO₂ electroreduction lowered on strained penta-twinned Cu nanowires. Chemical Science, 2015, 6, 6829-6835.	3.7	60

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37	First-principles simulations of exciton diffusion in organic semiconductors. Physical Review B, 2011, 84, .	1.1	58
38	Ordered PdCuâ€Based Nanoparticles as Bifunctional Oxygenâ€Reduction and Ethanolâ€Oxidation Electrocatalysts. Angewandte Chemie, 2016, 128, 9176-9181.	1.6	56
39	Shedding light on moirÃ© excitons: A first-principles perspective. Science Advances, 2020, 6, .	4.7	50
40	Charge Separation and Exciton Dynamics at Polymer/ZnO Interface from First-Principles Simulations. Journal of Physical Chemistry Letters, 2014, 5, 2649-2656.	2.1	48
41	Atomically Isolated Rh Sites within Highly Branched Rh₂Sb Nanostructures Enhance Bifunctional Hydrogen Electrocatalysis. Advanced Materials, 2021, 33, e2105049.	11.1	48
42	Excitonic Effect Drives Ultrafast Dynamics in van der Waals Heterostructures. Nano Letters, 2020, 20, 4631-4637.	4.5	46
43	Band Alignment in Two-Dimensional Halide Perovskite Heterostructures: Type I or Type II?. Journal of Physical Chemistry Letters, 2020, 11, 2910-2916.	2.1	43
44	Size-Dependent Plasmonic Resonances from Large-Scale Quantum Simulations. Journal of Physical Chemistry Letters, 2014, 5, 1163-1169.	2.1	41
45	Quantum simulation of materials at micron scales and beyond. Physical Review B, 2008, 78, .	1.1	33
46	Multiscale quantum/atomistic coupling using constrained density functional theory. Physical Review B, 2013, 87, .	1.1	32
47	Highly Surface-Distorted Pt Superstructures for Multifunctional Electrocatalysis. Nano Letters, 2021, 21, 5075-5082.	4.5	31
48	Effect of Point Defects on Optical Properties of Graphene Fluoride: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 12855-12862.	1.5	30
49	Tungstenâ€Đoped L1 0 â€PtCo Ultrasmall Nanoparticles as a Highâ€Performance Fuel Cell Cathode. Angewandte Chemie, 2019, 131, 15617-15623.	1.6	30
50	Understanding Quantum Plasmonics from Time-Dependent Orbital-Free Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 14330-14336.	1.5	29
51	Vacancy-induced MnO₆ distortion and its impacts on structural transition of Li₂MnO₃. Physical Chemistry Chemical Physics, 2017, 19, 7025-7031.	1.3	29
52	Modeling Auger Processes with Nonadiabatic Molecular Dynamics. Nano Letters, 2021, 21, 756-761.	4.5	29
53	Electron Dynamics in Dye-Sensitized Solar Cells: Effects of Surface Terminations and Defects. Journal of Physical Chemistry B, 2010, 114, 17077-17083.	1.2	28
54	Dynamic kinetic energy potential for orbital-free density functional theory. Journal of Chemical Physics, 2011, 134, 144101.	1.2	27

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55	Quantum mechanical modeling of hydrogen assisted cracking in aluminum. Physical Review B, 2013, 88, .	1.1	27
56	Decreasing Exciton Binding Energy in Two-Dimensional Halide Perovskites by Lead Vacancies. Journal of Physical Chemistry Letters, 2019, 10, 3820-3827.	2.1	27
57	First-principles determination of charge carrier mobility in disordered semiconducting polymers. Physical Review B, 2010, 82, .	1.1	26
58	Dipole-Assisted Charge Separation in Organicâ€“Inorganic Hybrid Photovoltaic Heterojunctions: Insight from First-Principles Simulations. Journal of Physical Chemistry C, 2012, 116, 9845-9851.	1.5	25
59	Subspace formulation of time-dependent density functional theory for large-scale calculations. Journal of Chemical Physics, 2015, 143, 064110.	1.2	24
60	Intramolecular Band Alignment and Spinâ€“Orbit Coupling in Two-Dimensional Halide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 6982-6989.	2.1	24
61	Self-Healing of Photocurrent Degradation in Perovskite Solar Cells: The Role of Defect-Trapped Excitons. Journal of Physical Chemistry Letters, 2019, 10, 7774-7780.	2.1	23
62	Charge transport in hybrid halide perovskites. Physical Review B, 2017, 96, .	1.1	22
63	Hole Transport in Diketopyrrolopyrrole (DPP) Small Molecules: A Joint Theoretical and Experimental Study. Journal of Physical Chemistry C, 2013, 117, 6730-6740.	1.5	21
64	Optically inactive defects in monolayer and bilayer phosphorene: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	21
65	A non-self-consistent range-separated time-dependent density functional approach for large-scale simulations. Journal of Physics Condensed Matter, 2012, 24, 205801.	0.7	20
66	Linear-Response Time-Dependent Density Functional Theory with Stochastic Range-Separated Hybrids. Journal of Chemical Theory and Computation, 2020, 16, 1064-1072.	2.3	19
67	Data driven discovery of conjugated polyelectrolytes for optoelectronic and photocatalytic applications. Npj Computational Materials, 2021, 7, .	3.5	19
68	Charge separation boosts exciton diffusion in fused ring electron acceptors. Journal of Materials Chemistry A, 2020, 8, 23304-23312.	5.2	18
69	Exclusive Strain Effect Boosts Overall Water Splitting in PdCu/Ir Core/Shell Nanocrystals. Angewandte Chemie, 2021, 133, 8324-8331.	1.6	18
70	The lowest-energy charge-transfer state and its role in charge separation in organic photovoltaics. Physical Chemistry Chemical Physics, 2016, 18, 17546-17556.	1.3	17
71	Unraveling Structural and Optical Properties of Two-Dimensional Mo_xW_{1â€“x}S₂ Alloys. Journal of Physical Chemistry C, 2021, 125, 774-781.	1.5	17
72	Dislocation cross-slip mechanisms in aluminum. Philosophical Magazine, 2011, 91, 4109-4125.	0.7	16

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73	MoirÃ© excitons in defective van der Waals heterostructures. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	16
74	Unraveling energy and charge transfer in type-II van der Waals heterostructures. Npj Computational Materials, 2021, 7, .	3.5	16
75	Electronic structure analysis of self-consistent embedding theory for quantum/molecular mechanics simulations. Physical Review B, 2008, 78, .	1.1	14
76	Charge Stripe Formation in Molecular Ferroelectric Organohalide Perovskites for Efficient Charge Separation. Journal of Physical Chemistry C, 2016, 120, 23969-23975.	1.5	14
77	Bimetallenes for selective electrocatalytic conversion of CO₂: a first-principles study. Journal of Materials Chemistry A, 2020, 8, 12457-12462.	5.2	14
78	Strongly Interacting C₆₀/Ir(111) Interface: Transformation of C₆₀ into Graphene and Influence of Graphene Interlayer. Journal of Physical Chemistry C, 2015, 119, 27550-27555.	1.5	13
79	Atomistic understanding of structural evolution, ion transport and oxygen stability in layered NaFeO₂. Journal of Materials Chemistry A, 2019, 7, 2619-2625.	5.2	13
80	Quantum Plasmonics in Nanorods: A Time-Dependent Orbital-Free Density Functional Theory Study with Thousands of Atoms. Journal of Physical Chemistry C, 2020, 124, 945-951.	1.5	13
81	Reducing Anomalous Hysteresis in Perovskite Solar Cells by Suppressing the Interfacial Ferroelectric Order. ACS Applied Materials & Interfaces, 2020, 12, 12275-12284.	4.0	13
82	Unraveling photoexcitation dynamics at â€œdots-in-a-perovskiteâ€•heterojunctions from first-principles. Journal of Materials Chemistry A, 2019, 7, 18012-18019.	5.2	12
83	Charge carrier mobility in a two-phase disordered organic system in the low-carrier concentration regime. Physical Review B, 2013, 88, .	1.1	11
84	Density-gradient-corrected embedded atom method. Physical Review B, 2009, 79, .	1.1	9
85	Controlling catalytic activity of gold cluster on MgO thin film for water splitting. Physical Review Materials, 2017, 1, .	0.9	9
86	Circumventing the scaling relationship on bimetallic monolayer electrocatalysts for selective CO₂ reduction. Chemical Science, 2022, 13, 3880-3887.	3.7	9
87	First-Principles Study of Electron Mobility in Cationic and Anionic Conjugated Polyelectrolytes. Journal of Physical Chemistry C, 2012, 116, 1205-1210.	1.5	8
88	Comment on â€œLinear Scaling of the Exciton Binding Energy versus the Band Gap of Two-Dimensional Materialsâ€• Physical Review Letters, 2017, 118, 209701.	2.9	8
89	First-order nonadiabatic couplings in extended systems by time-dependent density functional theory. Journal of Chemical Physics, 2018, 149, 244103.	1.2	8
90	Understanding molecular structure dependence of exciton diffusion in conjugated small molecules. Applied Physics Letters, 2014, 104, 143303.	1.5	7

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91	One-Dimensional Flat Bands and Anisotropic MoirÃ© Excitons in Twisted Tin Sulfide Bilayers. Chemistry of Materials, 2021, 33, 7432-7440.	3.2	6
92	Oxygen Reduction: Biaxial Strains Mediated Oxygen Reduction Electrocatalysis on Fenton Reaction Resistant L1‹sub›0‹/sub›â€Pt3Zn Fuel Cell Cathode (Adv. Energy Mater. 29/2020). Advanced Energy Materials, 2020, 10, 2070124.	10.2	5
93	Predictions of moirÃ© excitons in twisted two-dimensional organicâ€“inorganic halide perovskites. Chemical Science, 2021, 12, 6073-6080.	3.7	5
94	Coupled quantum mechanics/molecular mechanics modeling of metallic materials: Theory and applications. Journal of Materials Research, 2018, 33, 796-812.	1.2	4
95	Chemical tuning of band alignments for Cu/HfO2 interfaces. Physica Status Solidi (B): Basic Research, 2015, 252, 298-304.	0.7	3
96	Understanding Quantum Plasmonic Enhancement in Nanorod Dimers from Time-Dependent Orbital-Free Density Functional Theory. Journal of Physical Chemistry C, 2022, 126, 5046-5054.	1.5	3
97	Monte Carlo Simulations of Grain Boundary Sliding and Migration: Effect of Temperature and Vacancy. Materials Research Society Symposia Proceedings, 2000, 634, 3141.	0.1	2
98	Ab Initio Electronic Structure Calculations of the Î£ 5 (210) [001] Tilt Grain Boundary in Ni3Al. Materials Research Society Symposia Proceedings, 1997, 472, 21.	0.1	1