Xin Tan

List of Publications by Year
in descending order

109 papers	5,351 citations	66315 42 h-index	88593 70 g-index
110 all docs	110 docs citations	110 times ranked	6368 citing authors

#	Article	IF	Citations
1	Isolated Diatomic Niâ€Fe Metalâ€“Nitrogen Sites for Synergistic Electroreduction of CO₂. Angewandte Chemie - International Edition, 2019, 58, 6972-6976.	7.2	707
2	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. Journal of Physical Chemistry C, 2015, 119, 6918-6922.	1.5	210
3	Direct insights into the role of epoxy groups on cobalt sites for acidic H2O2 production. Nature Communications, 2020, 11, 4181.	5.8	204
4	A Janus MoSSe monolayer: a superior and strain-sensitive gas sensing material. Journal of Materials Chemistry A, 2019, 7, 1099-1106.	5.2	187
5	Tuning electronic and optical properties of MoS₂monolayer via molecular charge transfer. Journal of Materials Chemistry A, 2014, 2, 16892-16897.	5.2	145
6	A single-Pt-atom-on-Ru-nanoparticle electrocatalyst for CO-resilient methanol oxidation. Nature Catalysis, 2022, 5, 231-237.	16.1	133
7	Intrinsic ORR Activity Enhancement of Pt Atomic Sites by Engineering the <i>d</i>â€Band Center via Local Coordination Tuning. Angewandte Chemie - International Edition, 2021, 60, 21911-21917.	7.2	132
8	Electroreduction of CO₂ to CO on a Mesoporous Carbon Catalyst with Progressively Removed Nitrogen Moieties. ACS Energy Letters, 2018, 3, 2292-2298.	8.8	129
9	Atomically Dispersed Indium Sites for Selective CO₂ Electroreduction to Formic Acid. ACS Nano, 2021, 15, 5671-5678.	7.3	121
10	Isolated copperâ€“tin atomic interfaces tuning electrocatalytic CO2 conversion. Nature Communications, 2021, 12, 1449.	5.8	119
11	Templateâ€Directed Rapid Synthesis of Pdâ€Based Ultrathin Porous Intermetallic Nanosheets for Efficient Oxygen Reduction. Angewandte Chemie - International Edition, 2021, 60, 10942-10949.	7.2	115
12	Implanting Ni-O-VOx sites into Cu-doped Ni for low-overpotential alkaline hydrogen evolution. Nature Communications, 2020, 11, 2720.	5.8	113
13	Controllable CO2 electrocatalytic reduction via ferroelectric switching on single atom anchored In2Se3 monolayer. Nature Communications, 2021, 12, 5128.	5.8	110
14	Phosphine vapor-assisted construction of heterostructured Ni₂P/NiTe₂ catalysts for efficient hydrogen evolution. Energy and Environmental Science, 2020, 13, 1799-1807.	15.6	105
15	Sulfurâ€Dopantâ€Promoted Electroreduction of CO₂ over Coordinatively Unsaturated Niâ€N₂ Moieties. Angewandte Chemie - International Edition, 2021, 60, 23342-23348.	7.2	98
16	Modulating Pt-O-Pt atomic clusters with isolated cobalt atoms for enhanced hydrogen evolution catalysis. Nature Communications, 2022, 13, 2430.	5.8	98
17	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO₂ Reduction. Angewandte Chemie - International Edition, 2020, 59, 21493-21498.	7.2	97
18	Formation and Migration of Oxygen Vacancies in SrCoO₃ and Their Effect on Oxygen Evolution Reactions. ACS Catalysis, 2016, 6, 5565-5570.	5.5	96

#	Article	IF	Citations
19	Processable Surface Modification of Nickelâ€Heteroatom (N, S) Bridge Sites for Promoted Alkaline Hydrogen Evolution. Angewandte Chemie - International Edition, 2019, 58, 461-466.	7.2	95
20	Thermodynamic model of the surface energy of nanocrystals. Physical Review B, 2006, 74, .	1.1	89
21	Borophene as a Promising Material for Charge-Modulated Switchable CO₂ Capture. ACS Applied Materials & Interfaces, 2017, 9, 19825-19830.	4.0	83
22	N,P co-coordinated Fe species embedded in carbon hollow spheres for oxygen electrocatalysis. Journal of Materials Chemistry A, 2019, 7, 14732-14742.	5.2	80
23	On the mechanism of gas adsorption for pristine, defective and functionalized graphene. Physical Chemistry Chemical Physics, 2017, 19, 6051-6056.	1.3	73
24	Tungsten Oxide/Carbide Surface Heterojunction Catalyst with High Hydrogen Evolution Activity. ACS Energy Letters, 2020, 5, 3560-3568.	8.8	70
25	Interfacing BiVO 4 with Reduced Graphene Oxide for Enhanced Photoactivity: A Tale of Facet Dependence of Electron Shuttling. Small, 2016, 12, 5295-5302.	5.2	68
26	The controlled disassembly of mesostructured perovskites as an avenue to fabricating high performance nanohybrid catalysts. Nature Communications, 2017, 8, 15553.	5.8	65
27	Isolated Diatomic Niâ€Fe Metalâ€"Nitrogen Sites for Synergistic Electroreduction of CO₂. Angewandte Chemie, 2019, 131, 7046-7050.	1.6	65
28	Metallic BSi₃ Silicene: A Promising High Capacity Anode Material for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2014, 118, 25836-25843.	1.5	62
29	p-Doped Graphene/Graphitic Carbon Nitride Hybrid Electrocatalysts: Unraveling Charge Transfer Mechanisms for Enhanced Hydrogen Evolution Reaction Performance. ACS Catalysis, 2016, 6, 7071-7077.	5.5	62
30	First-principles study of structural, electronic, and multiferroic properties in BiCoO3. Journal of Chemical Physics, 2007, 126, 154708.	1.2	60
31	Conductive Graphitic Carbon Nitride as an Ideal Material for Electrocatalytically Switchable CO2 Capture. Scientific Reports, 2015, 5, 17636.	1.6	60
32	The origin of low workfunctions in OH terminated MXenes. Nanoscale, 2017, 9, 7016-7020.	2.8	59
33	Electronic Regulation of Nickel Single Atoms by Confined Nickel Nanoparticles for Energyâ€Efficient CO₂ Electroreduction. Angewandte Chemie - International Edition, 2022, 61, .	7.2	57
34	Confinement of Ionic Liquids at Single-Ni-Sites Boost Electroreduction of CO₂ in Aqueous Electrolytes. ACS Catalysis, 2020, 10, 13171-13178.	5.5	54
35	An Ultra-Long-Life Flexible Lithiumâ€"Sulfur Battery with Lithium Cloth Anode and Polysulfone-Functionalized Separator. ACS Nano, 2021, 15, 1358-1369.	7.3	53
36	Conductive Boron-Doped Graphene as an Ideal Material for Electrocatalytically Switchable and High-Capacity Hydrogen Storage. ACS Applied Materials & Interfaces, 2016, 8, 32815-32822.	4.0	52

#	Article	IF	Citations
37	Understanding the high activity of mildly reduced graphene oxide electrocatalysts in oxygen reduction to hydrogen peroxide. Materials Horizons, 2019, 6, 1409-1415.	6.4	51
38	Regulating electron transfer over asymmetric low-spin Co(II) for highly selective electrocatalysis. Chem Catalysis, 2022, 2, 372-385.	2.9	50
39	Mobile Polaronic States in Î±-MoO₃: An ab Initio Investigation of the Role of Oxygen Vacancies and Alkali Ions. ACS Applied Materials & Interfaces, 2016, 8, 10911-10917.	4.0	49
40	Stacking-Dependent Interlayer Magnetic Coupling in 2D CrI₃/CrGeTe₃ Nanostructures for Spintronics. ACS Applied Nano Materials, 2020, 3, 1282-1288.	2.4	47
41	Antipoisoning Nickelâ€“Carbon Electrocatalyst for Practical Electrochemical CO₂ Reduction to CO. ACS Applied Energy Materials, 2019, 2, 8002-8009.	2.5	45
42	Layered Grapheneâ€“Hexagonal BN Nanocomposites: Experimentally Feasible Approach to Chargeâ€Induced Switchable CO₂ Capture. ChemSusChem, 2015, 8, 2987-2993.	3.6	43
43	Autocatalytic Surface Reductionâ€Assisted Synthesis of PtW Ultrathin Alloy Nanowires for Highly Efficient Hydrogen Evolution Reaction. Advanced Energy Materials, 2022, 12, .	10.2	40
44	Solid solubility limit in alloying nanoparticles. Nanotechnology, 2006, 17, 4257-4262.	1.3	38
45	Metallic BSi₃ Silicene and Its One-Dimensional Derivatives: Unusual Nanomaterials with Planar Aromatic <i>D</i>_{6<i>h</i>} Six-Membered Silicon Rings. Journal of Physical Chemistry C, 2014, 118, 25825-25835.	1.5	37
46	Charge Modulation in Graphitic Carbon Nitride as a Switchable Approach to Highâ€Capacity Hydrogen Storage. ChemSusChem, 2015, 8, 3626-3631.	3.6	37
47	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO₂ Reduction. Angewandte Chemie, 2020, 132, 21677-21682.	1.6	37
48	Physical and chemical origin of size-dependent spontaneous interfacial alloying of coreâ€“shell nanostructures. Chemical Physics Letters, 2006, 420, 65-70.	1.2	34
49	Tetragonal bismuth bilayer: a stable and robust quantum spin hall insulator. 2D Materials, 2015, 2, 045010.	2.0	34
50	Versatile electrocatalytic processes realized by Ni, Co and Fe alloyed core coordinated carbon shells. Journal of Materials Chemistry A, 2019, 7, 12154-12165.	5.2	34
51	Electrocatalytic Reduction of Carbon Dioxide to Methane on Single Transition Metal Atoms Supported on a Defective Boron Nitride Monolayer: First Principle Study. Advanced Theory and Simulations, 2019, 2, 1800094.	1.3	33
52	Encapsulated Silicene: A Robust Large-Gap Topological Insulator. ACS Applied Materials & Interfaces, 2015, 7, 19226-19233.	4.0	31
53	Sc and Nb dopants in SrCoO3 modulate electronic and vacancy structures for improved water splitting and SOFC cathodes. Energy Storage Materials, 2017, 9, 229-234.	9.5	31
54	First-principles study of pressure-induced metal-insulator transition in BiNiO3. Applied Physics Letters, 2007, 91, 101901.	1.5	29

#	Article	IF	Citations
55	Surface energy and shrinkage of a nanocavity. Applied Physics Letters, 2006, 89, 183104.	1.5	28
56	Charge-controlled switchable H2 storage on conductive borophene nanosheet. International Journal of Hydrogen Energy, 2019, 44, 20150-20157.	3.8	26
57	Hexagonal boron nitride and graphene in-plane heterostructures: An experimentally feasible approach to charge-induced switchable CO 2 capture. Chemical Physics, 2016, 478, 139-144.	0.9	25
58	Computational design of two-dimensional nanomaterials for charge modulated CO2/H2 capture and/or storage. Energy Storage Materials, 2017, 8, 169-183.	9.5	25
59	RhNi nanocatalyst: Spontaneous alloying and high activity for hydrogen generation from hydrous hydrazine. International Journal of Hydrogen Energy, 2016, 41, 6362-6368.	3.8	24
60	Charge-modulated permeability and selectivity in graphdiyne for hydrogen purification. Molecular Simulation, 2016, 42, 573-579.	0.9	24
61	Defect Engineering in Graphene-Confined Single-Atom Iron Catalysts for Room-Temperature Methane Conversion. Journal of Physical Chemistry C, 2021, 125, 12628-12635.	1.5	22
62	Materials design for electrocatalytic carbon capture. APL Materials, 2016, 4, .	2.2	20
63	Light, Catalyst, Activation: Boosting Catalytic Oxygen Activation Using a Light Pretreatment Approach. ACS Catalysis, 2017, 7, 3644-3653.	5.5	20
64	Processable Surface Modification of Nickelâ€Heteroatom (N, S) Bridge Sites for Promoted Alkaline Hydrogen Evolution. Angewandte Chemie, 2018, 131, 471.	1.6	19
65	Dependence of morphology of pulsed-laser deposited coatings on temperature: a kinetic Monte Carlo simulation. Surface and Coatings Technology, 2005, 197, 288-293.	2.2	18
66	First-Principle Framework for Total Charging Energies in Electrocatalytic Materials and Charge-Responsive Molecular Binding at Gasâ€"Surface Interfaces. ACS Applied Materials & Interfaces, 2016, 8, 10897-10903.	4.0	18
67	Pulsed-laser deposition of polycrystalline Ni films: A three-dimensional kinetic Monte Carlo simulation. Surface Science, 2005, 588, 175-183.	0.8	15
68	Ordering Fe nanowire on stepped Cu (111) surface. Applied Physics Letters, 2006, 88, 263116.	1.5	14
69	Giant Magneto-Optical Kerr Effects in Ferromagnetic Perovskite BiNiO₃ with Half-Metallic State. Journal of Physical Chemistry C, 2008, 112, 16638-16642.	1.5	13
70	With the same Clar formulas, do the two-dimensional sandwich nanostructures Xâ€"Crâ€"X (X = C4H,) Tj ETQq0 0 0 rgBT /Overlock 10	1.3	13
71	Synthesis, optical properties and theoretical modelling of discrete emitting states in doped silicon nanocrystals for bioimaging. Nanoscale, 2018, 10, 15600-15607.	2.8	13
72	Ab initio study of rumpled relaxation and core-level shift of barium titanate surface. Surface Science, 2007, 601, 1345-1350.	0.8	12

#	Article	IF	Citations
73	Nitrogen Doped Carbon Nanosheets Coupled Nickelâ€"Carbon Pyramid Arrays Toward Efficient Evolution of Hydrogen. Advanced Sustainable Systems, 2017, 1, 1700032.	2.7	12
74	Unveiling the role of carbon oxidation in irreversible degradation of atomically-dispersed FeN₄ moieties for proton exchange membrane fuel cells. Journal of Materials Chemistry A, 2021, 9, 8721-8729.	5.2	11
75	In Operando Selfâ€Healing of Perovskite Electrocatalysts: A Case Study of SrCoO₃ for the Oxygen Evolution Reaction. Particle and Particle Systems Characterization, 2017, 34, 1600280.	1.2	10
76	Theory-guided construction of electron-deficient sites via removal of lattice oxygen for the boosted electrocatalytic synthesis of ammonia. Nano Research, 2021, 14, 1457-1464.	5.8	10
77	Templateâ€Directed Rapid Synthesis of Pdâ€Based Ultrathin Porous Intermetallic Nanosheets for Efficient Oxygen Reduction. Angewandte Chemie, 2021, 133, 11037-11044.	1.6	9
78	Sulfurâ€Dopantâ€Promoted Electroreduction of CO 2 over Coordinatively Unsaturated Niâ€N 2 Moieties. Angewandte Chemie, 0, , .	1.6	9
79	New insights on the substantially reduced bandgap of bismuth layered perovskite oxide thin films. Journal of Materials Chemistry C, 2021, 9, 3161-3170.	2.7	9
80	Electronic Regulation of Nickel Single Atoms by Confined Nickel Nanoparticles for Energyâ€Efficient CO₂ Electroreduction. Angewandte Chemie, 2022, 134, .	1.6	9
81	First-principles study for the atomic structures and electronic properties of PbTiO3 oxygen-vacancies (001) surface. Surface Science, 2007, 601, 5412-5418.	0.8	8
82	Charge-modulated CO2 capture. Current Opinion in Electrochemistry, 2017, 4, 118-123.	2.5	8
83	Oxygen Electrocatalysis at Mn^{III}â€"O<i>_x</i>â€"C Hybrid Heterojunction: An Electronic Synergy or Cooperative Catalysis?. ACS Applied Materials & Interfaces, 2019, 11, 706-713.	4.0	7
84	Facile CO Oxidation on Oxygenâ€functionalized MXenes via the Marsâ€van Krevelen Mechanism. ChemCatChem, 2020, 12, 1007-1012.	1.8	7
85	Vanadium Oxide Clusters Decorated Metallic Cobalt Catalyst for Active Alkaline Hydrogen Evolution. Cell Reports Physical Science, 2020, 1, 100275.	2.8	7
86	Regioselective Oxidation of Strained Graphene for Controllable Synthesis of Nanoribbons. Journal of Physical Chemistry C, 2013, 117, 19160-19166.	1.5	6
87	Unraveling the Factors Behind the Efficiency of Hydrogen Evolution in Endohedrally Doped C₆₀ Structures via Ab Initio Calculations and Insights from Machine Learning Models. Advanced Theory and Simulations, 2019, 2, 1800202.	1.3	6
88	Huge Lithium Storage in 2D Bilayer Structures with Point Defects. Journal of Physical Chemistry C, 2021, 125, 23597-23603.	1.5	6
89	Catalytic Bond-Breaking Selectivity in the Ethylene Decomposition on Ni Surfaces:â€‰ Kinetic Monte Carlo Simulations. Journal of Physical Chemistry C, 2008, 112, 4219-4225.	1.5	5
90	Enhanced stability and stacking dependent magnetic/electronic properties of 2D monolayer FeTiO₃ on a Ti₂CO₂ substrate. Journal of Materials Chemistry C, 2019, 7, 15308-15314.	2.7	5

#	Article	IF	Citations
91	Roughing titanium quantum wire on patterned monohydride diamond (001) surface. Journal of Chemical Physics, 2007, 126, 184705.	1.2	4
92	Supramolecular Nanowires Self-Assembly on Stepped Ag(110) Surface. Journal of Physical Chemistry C, 2009, 113, 19926-19929.	1.5	4
93	Intrinsic ORR Activity Enhancement of Pt Atomic Sites by Engineering the d â€Band Center via Local Coordination Tuning. Angewandte Chemie, 2021, 133, 22082-22088.	1.6	4
94	Plate model to evaluate interfacial adhesion of anisotropy thin film in CSN test. Journal of Materials Science, 2004, 39, 4013-4016.	1.7	2
95	Temperature-dependent surface alloying in Au/Ni (1 1 0). Journal of Alloys and Compounds, 2009, 467, 428-433.	2.8	2
96	Molecular dynamics study of temperature-dependent ripples in monolayer and bilayer graphene on 6Hâ€"SiC surfaces. Chinese Physics B, 2012, 21, 066803.	0.7	2
97	First-principles calculations of surfactant-assisted growth of polar CaO(111) oxide film: The case of water-based surfactant. Physical Review B, 2012, 86, .	1.1	2
98	Fermi Level Determination for Charged Systems via Recursive Density of States Integration. Journal of Physical Chemistry Letters, 2018, 9, 4014-4019.	2.1	2
99	Hydrophilic tannic acid-modified WS₂ nanosheets for enhanced polysulfide conversion in aqueous media. JPhys Energy, 2019, 1, 015005.	2.3	2
100	Activating Inert MXenes for Hydrogen Evolution Reaction via Anchored Metal Centers. Advanced Theory and Simulations, 2022, 5, .	1.3	2
101	COMPARISON OF ISLAND FORMATION BETWEEN PULSED LASER DEPOSITION AND MOLECULAR BEAM EPITAXY: A KINETIC MONTE CARLO SIMULATION. Surface Review and Letters, 2005, 12, 611-617.	0.5	1
102	Charge-induced transition between miscible and immiscible in nanometer-sized alloying particles. Chemical Physics Letters, 2006, 423, 143-146.	1.2	1
103	Thermodynamic stability of quantum dots on strained substrates. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1755-1758.	1.3	1
104	GROWTH MECHANISM OF RING SHAPED NANOSTRUCTURES SELF-ASSEMBLY UPON DROPLET EPITAXY. Surface Review and Letters, 2012, 19, 1250029.	0.5	1
105	Electrocatalysts: In Operando Self-Healing of Perovskite Electrocatalysts: A Case Study of SrCoO3 for the Oxygen Evolution Reaction (Part. Part. Syst. Charact. 4/2017). Particle and Particle Systems Characterization, 2017, 34, .	1.2	1
106	Computational Materials Science: Discovering and Accelerating Future Technologies. Advanced Theory and Simulations, 2019, 2, 1900023.	1.3	1
107	Photocatalysis: Interfacing BiVO₄ with Reduced Graphene Oxide for Enhanced Photoactivity: A Tale of Facet Dependence of Electron Shuttling (Small 38/2016). Small, 2016, 12, 5232-5232.	5.2	0
108	Hexagonal honeycomb silicon: Silicene. , 2017, , 171-188.		0

#	Article	IF	Citations
109	Hexagonal honeycomb silicon: Silicene. Series in Materials Science and Engineering, 2017, , 171-188.	0.1	0