Xin Tan

List of Publications by Citations

105	3,055	31	52
papers	citations	h-index	g-index
110	4,098	8.5	5.8
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
105	Isolated Diatomic Ni-Fe Metal-Nitrogen Sites for Synergistic Electroreduction of CO. *Angewandte Chemie - International Edition*, **2019**, 58, 6972-6976	16.4	406
104	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. *Journal of Physical Chemistry C*, **2015**, 119, 6918-6922	3.8	184
103	Tuning electronic and optical properties of MoS2 monolayer via molecular charge transfer. *Journal of Materials Chemistry A*, **2014**, 2, 16892-16897	13	123
102	A Janus MoSSe monolayer: a superior and strain-sensitive gas sensing material. *Journal of Materials Chemistry A*, **2019**, 7, 1099-1106	13	106
101	Thermodynamic model of the surface energy of nanocrystals. *Physical Review B*, **2006**, 74,	3.3	83
100	Electroreduction of CO2 to CO on a Mesoporous Carbon Catalyst with Progressively Removed Nitrogen Moieties. *ACS Energy Letters*, **2018**, 3, 2292-2298	20.1	78
99	Processable Surface Modification of Nickel-Heteroatom (N, S) Bridge Sites for Promoted Alkaline Hydrogen Evolution. *Angewandte Chemie - International Edition*, **2019**, 58, 461-466	16.4	74
98	Direct insights into the role of epoxy groups on cobalt sites for acidic HO production. *Nature Communications*, **2020**, 11, 4181	17.4	73
97	Formation and Migration of Oxygen Vacancies in SrCoO3 and Their Effect on Oxygen Evolution Reactions. *ACS Catalysis*, **2016**, 6, 5565-5570	13.1	66
96	Implanting Ni-O-VOx sites into Cu-doped Ni for low-overpotential alkaline hydrogen evolution. *Nature Communications*, **2020**, 11, 2720	17.4	65
95	Borophene as a Promising Material for Charge-Modulated Switchable CO Capture. *ACS Applied Materials & Interfaces*, **2017**, 9, 19825-19830	9.5	62
94	Phosphine vapor-assisted construction of heterostructured Ni2P/NiTe2 catalysts for efficient hydrogen evolution. *Energy and Environmental Science*, **2020**, 13, 1799-1807	35.4	56
93	Interfacing BiVO with Reduced Graphene Oxide for Enhanced Photoactivity: A Tale of Facet Dependence of Electron Shuttling. *Small*, **2016**, 12, 5295-5302	11	56
92	p-Doped Graphene/Graphitic Carbon Nitride Hybrid Electrocatalysts: Unraveling Charge Transfer Mechanisms for Enhanced Hydrogen Evolution Reaction Performance. *ACS Catalysis*, **2016**, 6, 7071-7077	13.1	53
91	The controlled disassembly of mesostructured perovskites as an avenue to fabricating high performance nanohybrid catalysts. *Nature Communications*, **2017**, 8, 15553	17.4	52
90	Metallic BSi3 Silicene: A Promising High Capacity Anode Material for Lithium-Ion Batteries. *Journal of Physical Chemistry C*, **2014**, 118, 25836-25843	3.8	52
89	First-principles study of structural, electronic, and multiferroic properties in BiCoO3. *Journal of Chemical Physics*, **2007**, 126, 154708	3.9	52

88	On the mechanism of gas adsorption for pristine, defective and functionalized graphene. *Physical Chemistry Chemical Physics*, **2017**, 19, 6051-6056	3.6	51
87	N,P co-coordinated Fe species embedded in carbon hollow spheres for oxygen electrocatalysis. *Journal of Materials Chemistry A*, **2019**, 7, 14732-14742	13	50
86	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO Reduction. *Angewandte Chemie - International Edition*, **2020**, 59, 21493-21498	16.4	50
85	Conductive Graphitic Carbon Nitride as an Ideal Material for Electrocatalytically Switchable CO2 Capture. *Scientific Reports*, **2015**, 5, 17636	4.9	48
84	Isolated Diatomic Ni-Fe Metal–Nitrogen Sites for Synergistic Electroreduction of CO2. *Angewandte Chemie*, **2019**, 131, 7046-7050	3.6	42
83	Conductive Boron-Doped Graphene as an Ideal Material for Electrocatalytically Switchable and High-Capacity Hydrogen Storage. *ACS Applied Materials & Interfaces*, **2016**, 8, 32815-32822	9.5	40
82	Mobile Polaronic States in □MoO3: An ab Initio Investigation of the Role of Oxygen Vacancies and Alkali Ions. *ACS Applied Materials & Interfaces*, **2016**, 8, 10911-7	9.5	40
81	Atomically Dispersed Indium Sites for Selective CO Electroreduction to Formic Acid. *ACS Nano*, **2021**, 15, 5671-5678	16.7	38
80	Layered Graphene-Hexagonal BN Nanocomposites: Experimentally Feasible Approach to Charge-Induced Switchable CO2 Capture. *ChemSusChem*, **2015**, 8, 2987-93	8.3	37
79	Solid solubility limit in alloying nanoparticles. *Nanotechnology*, **2006**, 17, 4257-62	3.4	36
78	Isolated copper-tin atomic interfaces tuning electrocatalytic CO conversion. *Nature Communications*, **2021**, 12, 1449	17.4	36
77	The origin of low workfunctions in OH terminated MXenes. *Nanoscale*, **2017**, 9, 7016-7020	7.7	35
76	Template-Directed Rapid Synthesis of Pd-Based Ultrathin Porous Intermetallic Nanosheets for Efficient Oxygen Reduction. *Angewandte Chemie - International Edition*, **2021**, 60, 10942-10949	16.4	35
75	Physical and chemical origin of size-dependent spontaneous interfacial alloying of core□shell nanostructures. *Chemical Physics Letters*, **2006**, 420, 65-70	2.5	33
74	Metallic BSi3 Silicene and Its One-Dimensional Derivatives: Unusual Nanomaterials with Planar Aromatic D6h Six-Membered Silicon Rings. *Journal of Physical Chemistry C*, **2014**, 118, 25825-25835	3.8	31
73	Understanding the high activity of mildly reduced graphene oxide electrocatalysts in oxygen reduction to hydrogen peroxide. *Materials Horizons*, **2019**, 6, 1409-1415	14.4	30
72	Controllable CO electrocatalytic reduction via ferroelectric switching on single atom anchored InSe monolayer. *Nature Communications*, **2021**, 12, 5128	17.4	30
71	Tetragonal bismuth bilayer: a stable and robust quantum spin hall insulator. *2D Materials*, **2015**, 2, 045010	7.9	29

70	Encapsulated Silicene: A Robust Large-Gap Topological Insulator. *ACS Applied Materials & Interfaces*, **2015**, 7, 19226-33	9.5	28
69	Charge Modulation in Graphitic Carbon Nitride as a Switchable Approach to High-Capacity Hydrogen Storage. *ChemSusChem*, **2015**, 8, 3626-31	8.3	27
68	Surface energy and shrinkage of a nanocavity. *Applied Physics Letters*, **2006**, 89, 183104	3.4	27
67	Stacking-Dependent Interlayer Magnetic Coupling in 2D CrI3/CrGeTe3 Nanostructures for Spintronics. *ACS Applied Nano Materials*, **2020**, 3, 1282-1288	5.6	27
66	Tungsten Oxide/Carbide Surface Heterojunction Catalyst with High Hydrogen Evolution Activity. *ACS Energy Letters*, **2020**, 5, 3560-3568	20.1	27
65	Confinement of Ionic Liquids at Single-Ni-Sites Boost Electroreduction of CO2 in Aqueous Electrolytes. *ACS Catalysis*, **2020**, 10, 13171-13178	13.1	27
64	Antipoisoning Nickel□arbon Electrocatalyst for Practical Electrochemical CO2 Reduction to CO. *ACS Applied Energy Materials*, **2019**, 2, 8002-8009	6.1	26
63	First-principles study of pressure-induced metal-insulator transition in BiNiO3. *Applied Physics Letters*, **2007**, 91, 101901	3.4	26
62	Intrinsic ORR Activity Enhancement of Pt Atomic Sites by Engineering the d-Band Center via Local Coordination Tuning. *Angewandte Chemie - International Edition*, **2021**, 60, 21911-21917	16.4	24
61	RhNi nanocatalyst: Spontaneous alloying and high activity for hydrogen generation from hydrous hydrazine. *International Journal of Hydrogen Energy*, **2016**, 41, 6362-6368	6.7	23
60	Versatile electrocatalytic processes realized by Ni, Co and Fe alloyed core coordinated carbon shells. *Journal of Materials Chemistry A*, **2019**, 7, 12154-12165	13	22
59	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	3.5	22
58	Computational design of two-dimensional nanomaterials for charge modulated CO2/H2 capture and/or storage. *Energy Storage Materials*, **2017**, 8, 169-183	19.4	21
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	2.3	21
56	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO2 Reduction. *Angewandte Chemie*, **2020**, 132, 21677-21682	3.6	20
55	An Ultra-Long-Life Flexible Lithium-Sulfur Battery with Lithium Cloth Anode and Polysulfone-Functionalized Separator. *ACS Nano*, **2021**, 15, 1358-1369	16.7	19
54	Charge-modulated permeability and selectivity in graphdiyne for hydrogen purification. *Molecular Simulation*, **2016**, 42, 573-579	2	18
53	Materials design for electrocatalytic carbon capture. *APL Materials*, **2016**, 4, 053202	5.7	18

52	Light, Catalyst, Activation: Boosting Catalytic Oxygen Activation Using a Light Pretreatment Approach. *ACS Catalysis*, **2017**, 7, 3644-3653	13.1	17
51	Charge-controlled switchable H2 storage on conductive borophene nanosheet. *International Journal of Hydrogen Energy*, **2019**, 44, 20150-20157	6.7	17
50	Dependence of morphology of pulsed-laser deposited coatings on temperature: a kinetic Monte Carlo simulation. *Surface and Coatings Technology*, **2005**, 197, 288-293	4.4	17
49	First-Principle Framework for Total Charging Energies in Electrocatalytic Materials and Charge-Responsive Molecular Binding at Gas-Surface Interfaces. *ACS Applied Materials & Interfaces*, **2016**, 8, 10897-903	9.5	16
48	Pulsed-laser deposition of polycrystalline Ni films: A three-dimensional kinetic Monte Carlo simulation. *Surface Science*, **2005**, 588, 175-183	1.8	15
47	Ordering Fe nanowire on stepped Cu (111) surface. *Applied Physics Letters*, **2006**, 88, 263116	3.4	14
46	Sulfur-Dopant-Promoted Electroreduction of CO over Coordinatively Unsaturated Ni-N Moieties. *Angewandte Chemie - International Edition*, **2021**, 60, 23342-23348	16.4	14
45	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	19.4	13
44	Ab initio study of rumpled relaxation and core-level shift of barium titanate surface. *Surface Science* , **2007**, 601, 1345-1350	1.8	12
43	Synthesis, optical properties and theoretical modelling of discrete emitting states in doped silicon nanocrystals for bioimaging. *Nanoscale*, **2018**, 10, 15600-15607	7.7	10
42	With the same Clar formulas, do the two-dimensional sandwich nanostructures X-Cr-X (X = C4H, NC3 and BC3) behave similarly?. *Physical Chemistry Chemical Physics*, **2014**, 16, 6002-11	3.6	10
41	In Operando Self-Healing of Perovskite Electrocatalysts: A Case Study of SrCoO3 for the Oxygen Evolution Reaction. *Particle and Particle Systems Characterization*, **2017**, 34, 1600280	3.1	9
40	Nitrogen Doped Carbon Nanosheets Coupled Nickel□arbon Pyramid Arrays Toward Efficient Evolution of Hydrogen. *Advanced Sustainable Systems*, **2017**, 1, 1700032	5.9	9
39	Giant Magneto-Optical Kerr Effects in Ferromagnetic Perovskite BiNiO3 with Half-Metallic State. *Journal of Physical Chemistry C*, **2008**, 112, 16638-16642	3.8	8
38	Regulating electron transfer over asymmetric low-spin Co(II) for highly selective electrocatalysis. *Chem Catalysis*, **2022**,		8
37	Defect Engineering in Graphene-Confined Single-Atom Iron Catalysts for Room-Temperature Methane Conversion. *Journal of Physical Chemistry C*, **2021**, 125, 12628-12635	3.8	8
36	A single-Pt-atom-on-Ru-nanoparticle electrocatalyst for CO-resilient methanol oxidation. *Nature Catalysis*, **2022**, 5, 231-237	36.5	8
35	First-principles study for the atomic structures and electronic properties of PbTiO3 oxygen-vacancies (001) surface. *Surface Science*, **2007**, 601, 5412-5418	1.8	7

34	Modulating Pt-O-Pt atomic clusters with isolated cobalt atoms for enhanced hydrogen evolution catalysis.. *Nature Communications*, **2022**, 13, 2430	17.4	7
33	Charge-modulated CO2 capture. *Current Opinion in Electrochemistry*, **2017**, 4, 118-123	7.2	6
32	Autocatalytic Surface Reduction-Assisted Synthesis of PtW Ultrathin Alloy Nanowires for Highly Efficient Hydrogen Evolution Reaction. *Advanced Energy Materials*,2103943	21.8	6
31	Oxygen Electrocatalysis at Mn-O -C Hybrid Heterojunction: An Electronic Synergy or Cooperative Catalysis?. *ACS Applied Materials & Interfaces*, **2019**, 11, 706-713	9.5	6
30	Catalytic Bond-Breaking Selectivity in the Ethylene Decomposition on Ni Surfaces: Kinetic Monte Carlo Simulations. *Journal of Physical Chemistry C*, **2008**, 112, 4219-4225	3.8	5
29	Regioselective Oxidation of Strained Graphene for Controllable Synthesis of Nanoribbons. *Journal of Physical Chemistry C*, **2013**, 117, 19160-19166	3.8	4
28	Supramolecular Nanowires Self-Assembly on Stepped Ag(110) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 19926-19929	3.8	4
27	Roughing titanium quantum wire on patterned monohydride diamond (001) surface. *Journal of Chemical Physics*, **2007**, 126, 184705	3.9	4
26	Template-Directed Rapid Synthesis of Pd-Based Ultrathin Porous Intermetallic Nanosheets for Efficient Oxygen Reduction. *Angewandte Chemie*, **2021**, 133, 11037-11044	3.6	4
25	Processable Surface Modification of Nickel-Heteroatom (N, S) Bridge Sites for Promoted Alkaline Hydrogen Evolution. *Angewandte Chemie*, **2018**, 131, 471	3.6	4
24	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	3.5	3
23	New insights on the substantially reduced bandgap of bismuth layered perovskite oxide thin films. *Journal of Materials Chemistry C*, **2021**, 9, 3161-3170	7.1	3
22	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	7.1	2
21	Molecular dynamics study of temperature-dependent ripples in monolayer and bilayer graphene on 6H-SiC surfaces. *Chinese Physics B*, **2012**, 21, 066803	1.2	2
20	First-principles calculations of surfactant-assisted growth of polar CaO(111) oxide film: The case of water-based surfactant. *Physical Review B*, **2012**, 86,	3.3	2
19	Temperature-dependent surface alloying in Au/Ni (110). *Journal of Alloys and Compounds*, **2009**, 467, 428-433	5.7	2
18	Plate model to evaluate interfacial adhesion of anisotropy thin film in CSN test. *Journal of Materials Science*, **2004**, 39, 4013-4016	4.3	2
17	Vanadium Oxide Clusters Decorated Metallic Cobalt Catalyst for Active Alkaline Hydrogen Evolution. *Cell Reports Physical Science*, **2020**, 1, 100275	6.1	2

List of Publications

16	Facile CO Oxidation on Oxygen-functionalized MXenes via the Mars-van Krevelen Mechanism. *ChemCatChem*, **2020**, 12, 1007-1012	5.2	2
15	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	10	2
14	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	13	2
13	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,	3.1	1
12	GROWTH MECHANISM OF RING SHAPED NANOSTRUCTURES SELF-ASSEMBLY UPON DROPLET EPITAXY. *Surface Review and Letters*, **2012**, 19, 1250029	1.1	1
11	Thermodynamic stability of quantum dots on strained substrates. *Physica E: Low-Dimensional Systems and Nanostructures*, **2011**, 43, 1755-1758	3	1
10	Charge-induced transition between miscible and immiscible in nanometer-sized alloying particles. *Chemical Physics Letters*, **2006**, 423, 143-146	2.5	1
9	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	1.1	1
8	Fermi Level Determination for Charged Systems via Recursive Density of States Integration. *Journal of Physical Chemistry Letters*, **2018**, 9, 4014-4019	6.4	1
7	Computational Materials Science: Discovering and Accelerating Future Technologies. *Advanced Theory and Simulations*, **2019**, 2, 1900023	3.5	0
6	Intrinsic ORR Activity Enhancement of Pt Atomic Sites by Engineering the d-Band Center via Local Coordination Tuning. *Angewandte Chemie*, **2021**, 133, 22082-22088	3.6	0
5	Hydrophilic tannic acid-modified WS2 nanosheets for enhanced polysulfide conversion in aqueous media. *JPhys Energy*, **2019**, 1, 015005	4.9	
4	Activating Inert MXenes for Hydrogen Evolution Reaction via Anchored Metal Centers. *Advanced Theory and Simulations*,2100383	3.5	
3	Hexagonal honeycomb silicon: Silicene **2017**, 171-188		
2	Hexagonal honeycomb silicon: Silicene. *Series in Materials Science and Engineering*, **2017**, 171-188		
1	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	11	