Yuzheng Guo

List of Publications by Year in descending order

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106 papers	4,098 citations	126907 33 h-index	128289 60 g-index
106 all docs	106 docs citations	106 times ranked	4933 citing authors

#	Article	IF	Citations
1	Impact of carbonâ€“carbon defects at the SiO₂/4H-SiC (0001) interface: a first-principles calculation. Journal Physics D: Applied Physics, 2022, 55, 025109.	2.8	4
2	MoirÃ© flat bands in twisted 2D hexagonal vdW materials. 2D Materials, 2022, 9, 014005.	4.4	10
3	Identifying TM-N4 active sites for selective CO2-to-CH4 conversion: A computational study. Applied Surface Science, 2022, 582, 152470.	6.1	16
4	p-Type Semiconduction in Oxides with Cation Lone Pairs. Chemistry of Materials, 2022, 34, 643-651.	6.7	12
5	Negative Differential Resistance Effect in â€œColdâ€•Metal Heterostructure Diodes. IEEE Electron Device Letters, 2022, 43, 498-501.	3.9	8
6	(In_xGa_{1â^’}_x)₂O₃ Thin Film Based Solarâ€Blind Deep UV Photodetectors with Ultraâ€High Detectivity and On/Off Current Ratio. Advanced Optical Materials, 2022, 10, .	7.3	16
7	An aqueous zincâ€ion battery working at â^’50Â°C enabled by lowâ€concentration perchlorateâ€based chaotropic salt electrolyte. EcoMat, 2022, 4, .	11.9	40
8	Tuning Ni dopant concentration to enable co-deposited superhydrophilic self-standing Mo2C electrode for high-efficient hydrogen evolution reaction. Applied Catalysis B: Environmental, 2022, 307, 121201.	20.2	36
9	Reduced Fermi Level Pinning at Physisorptive Sites of Moire-MoS₂/Metal Schottky Barriers. ACS Applied Materials & Interfaces, 2022, 14, 11903-11909.	8.0	17
10	Computation-guided design and preparation of durable and efficient WC-Mo2C heterojunction for hydrogen evolution reaction. Cell Reports Physical Science, 2022, 3, 100784.	5.6	6
11	Large piezoelectricity response in Li and Ti (or Zr) co-alloyed w-AlN. Journal of Applied Physics, 2022, 131, .	2.5	1
12	Revealing the oxygen Reduction/Evolution reaction activity origin of Carbon-Nitride-Related Single-Atom catalysts: Quantum chemistry in artificial intelligence. Chemical Engineering Journal, 2022, 440, 135946.	12.7	35
13	An all two-dimensional vertical heterostructure graphene/CuInP₂S₆/MoS₂ for negative capacitance field effect transistor. Nanotechnology, 2022, 33, 125703.	2.6	11
14	Self-Poisoning by C₂ Products in CO₂ Photoreduction Using a Phosphorus-Doped Carbon Nitride with Nitrogen Vacancies. ACS Sustainable Chemistry and Engineering, 2022, 10, 5758-5769.	6.7	14
15	Two-dimensional metalâ€“organic frameworks as efficient electrocatalysts for bifunctional oxygen evolution/reduction reactions. Journal of Materials Chemistry A, 2022, 10, 13005-13012.	10.3	21
16	Strain-promoted conductive metal-benzenehexathiolate frameworks for overall water splitting. Journal of Colloid and Interface Science, 2022, 624, 160-167.	9.4	10
17	Impact of Coordination Environment on Single-Atom-Embedded C₃N for Oxygen Electrocatalysis. ACS Sustainable Chemistry and Engineering, 2022, 10, 7692-7701.	6.7	14
18	Electronic properties of CaF2 bulk and interfaces. Journal of Applied Physics, 2022, 131, .	2.5	8

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19	Theoretical Insights into the Mechanism of Selective Nitrateâ€toâ€Ammonia Electroreduction on Singleâ€Atom Catalysts. Advanced Functional Materials, 2021, 31, 2008533.	14.9	240
20	Defects and Passivation Mechanism of the Suboxide Layers at SiOâ„/4H-SiC (0001) Interface: A First-Principles Calculation. IEEE Transactions on Electron Devices, 2021, 68, 288-293.	3.0	13
21	An Atomically Thin Airâ€Stable Narrowâ€Gap Semiconductor Cr₂S₃ for Broadband Photodetection with High Responsivity. Advanced Electronic Materials, 2021, 7, 2000962.	5.1	22
22	Carbon cluster formation and mobility degradation in 4H-SiC MOSFETs. Applied Physics Letters, 2021, 118, .	3.3	18
23	Tellurium Nanowire Gate-All-Around MOSFETs for Sub-5 nm Applications. ACS Applied Materials & Interfaces, 2021, 13, 3387-3396.	8.0	30
24	Iron Selenide Microcapsules as Universal Conversionâ€Typed Anodes for Alkali Metalâ€Ion Batteries. Small, 2021, 17, e2005745.	10.0	66
25	Single-Atom Rhodium on Defective g-C₃N₄: A Promising Bifunctional Oxygen Electrocatalyst. ACS Sustainable Chemistry and Engineering, 2021, 9, 3590-3599.	6.7	136
26	Electronic properties and tunability of the hexagonal SiGe alloys. Applied Physics Letters, 2021, 118, .	3.3	10
27	The Electrophilicity of Surface Carbon Species in the Redox Reactions of CuOâ€CeO 2 Catalysts. Angewandte Chemie, 2021, 133, 14541-14549.	2.0	2
28	Controllable High-Performance Memristors Based on 2D Fe2GeTe3 Oxide for Biological Synapse Imitation. Nanotechnology, 2021, 32, .	2.6	4
29	The Electrophilicity of Surface Carbon Species in the Redox Reactions of CuOâ€CeO₂ Catalysts. Angewandte Chemie - International Edition, 2021, 60, 14420-14428.	13.8	24
30	Schottky barrier heights of defect-free metal/ZnO, CdO, MgO, and SrO interfaces. Journal of Applied Physics, 2021, 129, .	2.5	14
31	Frontispiz: The Electrophilicity of Surface Carbon Species in the Redox Reactions of CuOâ€CeO₂ Catalysts. Angewandte Chemie, 2021, 133, .	2.0	0
32	Machine-Learning-Accelerated Catalytic Activity Predictions of Transition Metal Phthalocyanine Dual-Metal-Site Catalysts for CO₂ Reduction. Journal of Physical Chemistry Letters, 2021, 12, 6111-6118.	4.6	80
33	The metalâ€“insulator phase change in vanadium dioxide and its applications. Journal of Applied Physics, 2021, 129, .	2.5	25
34	Frontispiece: The Electrophilicity of Surface Carbon Species in the Redox Reactions of CuOâ€CeO₂ Catalysts. Angewandte Chemie - International Edition, 2021, 60, .	13.8	1
35	Two-Dimensional Gallium Oxide Monolayer for Gas-Sensing Application. Journal of Physical Chemistry Letters, 2021, 12, 5813-5820.	4.6	41
36	A Feasible Strategy for Identifying Singleâ€Atom Catalysts Toward Electrochemical NOâ€toâ€NH₃ Conversion. Small, 2021, 17, e2102396.	10.0	89

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37	A Marr's Threeâ€Level Analytical Framework for Neuromorphic Electronic Systems. Advanced Intelligent Systems, 2021, 3, 2100054.	6.1	3
38	Highâ€Throughput Electronic Structures and Ferroelectric Interfaces of HfO 2 by GGA+ U (d,p) Calculations. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100295.	2.4	5
39	A density-functional-theory-based and machine-learning-accelerated hybrid method for intricate system catalysis. Materials Reports Energy, 2021, 1, 100046.	3.2	13
40	Unraveling the Origin of Sulfurâ€Doped Feâ€Nâ€C Singleâ€Atom Catalyst for Enhanced Oxygen Reduction Activity: Effect of Iron Spinâ€State Tuning. Angewandte Chemie, 2021, 133, 25608-25614.	2.0	38
41	Ab Initio Study of Hexagonal Boron Nitride as the Tunnel Barrier in Magnetic Tunnel Junctions. ACS Applied Materials & Interfaces, 2021, 13, 47226-47235.	8.0	6
42	Unraveling the Origin of Sulfurâ€Doped Feâ€Nâ€C Singleâ€Atom Catalyst for Enhanced Oxygen Reduction Activity: Effect of Iron Spinâ€State Tuning. Angewandte Chemie - International Edition, 2021, 60, 25404-25410.	13.8	177
43	Blowing Iron Chalcogenides into Two-Dimensional Flaky Hybrids with Superior Cyclability and Rate Capability for Potassium-Ion Batteries. ACS Nano, 2021, 15, 2506-2519.	14.6	79
44	A new opportunity for the emerging tellurium semiconductor: making resistive switching devices. Nature Communications, 2021, 12, 6081.	12.8	25
45	Tunable contacts and device performances in graphene/group-III monochalcogenides MX (Mâ€‰=â€‰In, Ga;) Tj ETQq1 1 0.784314	2.5	8
46	A durable and pH-universal self-standing MoCâ€“Mo2C heterojunction electrode for efficient hydrogen evolution reaction. Nature Communications, 2021, 12, 6776.	12.8	169
47	Machineâ€learningâ€based interatomic potentials for advanced manufacturing. International Journal of Mechanical System Dynamics, 2021, 1, 159-172.	2.8	4
48	Impact of the interface vacancy on Schottky barrier height for Au/AlN polar interfaces. Applied Surface Science, 2020, 505, 144650.	6.1	15
49	A New Opportunity for 2D van der Waals Heterostructures: Making Steepâ€Slope Transistors. Advanced Materials, 2020, 32, e1906000.	21.0	82
50	Enhanced electrochemical oxygen evolution reaction activity on natural single-atom catalysts transition metal phthalocyanines: the substrate effect. Catalysis Science and Technology, 2020, 10, 8339-8346.	4.1	22
51	Extending the metal-induced gap state model of Schottky barriers. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2020, 38, .	1.2	14
52	Origin of Weaker Fermi Level Pinning and Localized Interface States at Metal Silicide Schottky Barriers. Journal of Physical Chemistry C, 2020, 124, 19698-19703.	3.1	11
53	Theoretical study on the photocatalytic properties of 2D InX(X = S, Se)/transition metal disulfide (MoS₂and WS₂) van der Waals heterostructures. Nanoscale, 2020, 12, 20025-20032.	5.6	49
54	Computational Screening Single-Atom Catalysts Supported on g-CN for N₂ Reduction: High Activity and Selectivity. ACS Sustainable Chemistry and Engineering, 2020, 8, 13749-13758.	6.7	167

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55	Role of the third metal oxide in Inâ€“Gaâ€“Znâ€“O4 amorphous oxide semiconductors: Alternatives to gallium. Journal of Applied Physics, 2020, 128, 215704.	2.5	6
56	Controllable Thermal Oxidation and Photoluminescence Enhancement in Quasi-1D van der Waals ZrS₃ Flakes. ACS Applied Electronic Materials, 2020, 2, 3756-3764.	4.3	12
57	Theoretical investigation on graphene-supported single-atom catalysts for electrochemical CO₂ reduction. Catalysis Science and Technology, 2020, 10, 8465-8472.	4.1	35
58	Modelling the enthalpy change and transition temperature dependence of the metalâ€“insulator transition in pure and doped vanadium dioxide. Physical Chemistry Chemical Physics, 2020, 22, 13474-13478.	2.8	12
59	Tuning the high-Î° oxide (HfO2, ZrO2)/4H-SiC interface properties with a SiO2 interlayer for power device applications. Applied Surface Science, 2020, 527, 146843.	6.1	13
60	Band Structure, Band Offsets, and Intrinsic Defect Properties of Few-Layer Arsenic and Antimony. Journal of Physical Chemistry C, 2020, 124, 7441-7448.	3.1	9
61	Revealing the oxygen reduction reaction activity origin of single atoms supported on g-C₃N₄ monolayers: a first-principles study. Journal of Materials Chemistry A, 2020, 8, 6555-6563.	10.3	140
62	Phase boundary engineering of metal-organic-framework-derived carbonaceous nickel selenides for sodium-ion batteries. Nano Research, 2020, 13, 2289-2298.	10.4	51
63	Termination-dependence of Fermi level pinning at rare-earth arsenide/GaAs interfaces. Applied Physics Letters, 2020, 116, .	3.3	6
64	Hybrid band offset calculation for heterojunction interfaces between disparate semiconductors. Applied Physics Letters, 2020, 116, .	3.3	9
65	Anisotropic Transport Property of Antimonene MOSFETs. ACS Applied Materials & Interfaces, 2020, 12, 22378-22386.	8.0	30
66	Phase dependence of Schottky barrier heights for Geâ€“Sbâ€“Te and related phase-change materials. Journal of Applied Physics, 2020, 127, .	2.5	7
67	Electronic structure of amorphous copper iodide: A <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -type transparent semiconductor. Physical Review Materials, 2020, 4, .	2.4	10
68	Effect of Phase Transition on Optical Properties and Photovoltaic Performance in Cesium Lead Bromine Perovskite: A Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 20764-20768.	3.1	2
69	Schottky barrier height at metal/ZnO interface: A first-principles study. Microelectronic Engineering, 2019, 216, 111056.	2.4	13
70	Band alignment calculation of dielectric films on VO2. Microelectronic Engineering, 2019, 216, 111057.	2.4	2
71	Structural changes during the switching transition of chalcogenide selector devices. Applied Physics Letters, 2019, 115, .	3.3	13
72	Atomic structure and band alignment at Al2O3/GaN, Sc2O3/GaN and La2O3/GaN interfaces: A first-principles study. Microelectronic Engineering, 2019, 216, 111039.	2.4	12

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73	Chemical bonding and band alignment at X2O3/GaN (Xâ€‰=â€‰Al, Sc) interfaces. Applied Physics Letters, 2019, 114, .	3.3	36
74	Electronic structure of metallic and insulating phases of vanadium dioxide and its oxide alloys. Physical Review Materials, 2019, 3, .	2.4	11
75	Band edge states, intrinsic defects, and dopants in monolayer HfS2 and SnS2. Applied Physics Letters, 2018, 112, .	3.3	22
76	Grapheneâ€“Organic Two-Dimensional Charge-Transfer Complexes: Intermolecular Electronic Transitions and Broadband Near-Infrared Photoresponse. Journal of Physical Chemistry C, 2018, 122, 7551-7556.	3.1	25
77	Oxygen vacancies and hydrogen in amorphous In-Ga-Zn-O and ZnO. Physical Review Materials, 2018, 2, .	2.4	21
78	Defect passivation of transition metal dichalcogenides via a charge transfer van der Waals interface. Science Advances, 2017, 3, e1701661.	10.3	95
79	Hydrogen and the Light-Induced Bias Instability Mechanism in Amorphous Oxide Semiconductors. Scientific Reports, 2017, 7, 16858.	3.3	19
80	Charge transfer doping of graphene without degrading carrier mobility. Journal of Applied Physics, 2017, 121, .	2.5	10
81	Photonic-plasmonic hybrid single-molecule nanosensor measures the effect of fluorescent labels on DNA-protein dynamics. Science Advances, 2017, 3, e1602991.	10.3	57
82	Face Dependence of Schottky Barriers Heights of Silicides and Germanides on Si and Ge. Scientific Reports, 2017, 7, 16669.	3.3	14
83	Band structure, band offsets, substitutional doping, and Schottky barriers of bulk and monolayer InSe. Physical Review Materials, 2017, 1, .	2.4	39
84	Band engineering in transition metal dichalcogenides: Stacked versus lateral heterostructures. Applied Physics Letters, 2016, 108, .	3.3	151
85	Chemical trends of Schottky barrier behavior on monolayer hexagonal B, Al, and Ga nitrides. Journal of Applied Physics, 2016, 120, .	2.5	13
86	Impact of oxygen exchange reaction at the ohmic interface in Ta₂O₅-based ReRAM devices. Nanoscale, 2016, 8, 17774-17781.	5.6	116
87	Interface Engineering for Atomic Layer Deposited Alumina Gate Dielectric on SiGe Substrates. ACS Applied Materials & Interfaces, 2016, 8, 19110-19118.	8.0	34
88	A fast transfer-free synthesis of high-quality monolayer graphene on insulating substrates by a simple rapid thermal treatment. Nanoscale, 2016, 8, 2594-2600.	5.6	20
89	Oxide defects and reliability of high K/Ge and IIIâ€“V based gate stacks. , 2015, , .		0
90	Localized Tail States and Electron Mobility in Amorphous ZnON Thin Film Transistors. Scientific Reports, 2015, 5, 13467.	3.3	70

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91	3D Behavior of Schottky Barriers of 2D Transition-Metal Dichalcogenides. ACS Applied Materials & Interfaces, 2015, 7, 25709-25715.	8.0	134
92	The effects of screening length in the non-local screened-exchange functional. Journal of Physics Condensed Matter, 2015, 27, 025501.	1.8	10
93	Comparison of oxygen vacancy defects in crystalline and amorphous Ta2O5. Microelectronic Engineering, 2015, 147, 254-259.	2.4	25
94	Calculation of TiO₂ Surface and Subsurface Oxygen Vacancy by the Screened Exchange Functional. Journal of Physical Chemistry C, 2015, 119, 18160-18166.	3.1	136
95	Ab initio calculations of materials selection of oxides for resistive random access memories. Microelectronic Engineering, 2015, 147, 339-343.	2.4	10
96	Selective Passivation of GeO₂/Ge Interface Defects in Atomic Layer Deposited High-k MOS Structures. ACS Applied Materials & Interfaces, 2015, 7, 20499-20506.	8.0	66
97	Efficient Transfer Doping of Carbon Nanotube Forests by MoO₃. ACS Nano, 2015, 9, 10422-10430.	14.6	39
98	Vacancy and Doping States in Monolayer and bulk Black Phosphorus. Scientific Reports, 2015, 5, 14165.	3.3	55
99	Materials selection for oxide-based resistive random access memories. Applied Physics Letters, 2014, 105, .	3.3	92
100	Origin of the high work function and high conductivity of MoO3. Applied Physics Letters, 2014, 105, .	3.3	161
101	Light induced instability mechanism in amorphous InGaZn oxide semiconductors. Applied Physics Letters, 2014, 104, .	3.3	60
102	Oxygen vacancy defects in Ta2O5 showing long-range atomic re-arrangements. Applied Physics Letters, 2014, 104, .	3.3	42
103	Calculation of metallic and insulating phases of V2O3 by hybrid density functionals. Journal of Chemical Physics, 2014, 140, 054702.	3.0	24
104	Chemical trends of defects at HfO2:GaAs and Al2O3:GaAs/InAs/InP/GaSb interfaces. Journal of Applied Physics, 2013, 113, .	2.5	22
105	Electrical conduction of carbon nanotube forests through sub-nanometric films of alumina. Applied Physics Letters, 2013, 102, .	3.3	24
106	Electronic and magnetic properties of Ti₂O₃, Cr₂O₃, and Fe₂O₃calculated by the screened exchange hybrid density functional. Journal of Physics Condensed Matter, 2012, 24, 325504.	1.8	82