Graeme A Henkelman

List of Publications by Year
in descending order

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291 papers	58,526 citations	9264 74 h-index	1009 236 g-index
300 all docs	300 docs citations	300 times ranked	38689 citing authors

#	Article	IF	Citations
1	A Sodiumâ€“Antimonyâ€“Telluride Intermetallic Allows Sodiumâ€Metal Cycling at 100% Depth of Discharge and as an Anodeâ€Free Metal Battery. Advanced Materials, 2022, 34, e2106005.	21.0	40
2	Theoretical study of structure sensitivity on Au doped CeO2 surfaces for formaldehyde oxidation: The effect of crystal planes and Au doping. Chemical Engineering Journal, 2022, 433, 133599.	12.7	7
3	Gold boosts nitrate reduction and deactivation resistance to indium-promoted palladium catalysts. Applied Catalysis B: Environmental, 2022, 305, 121048.	20.2	29
4	Green self-derived templating preparation of nitrogen, sulfur co-doped porous carbon/tin composites with synergistic effect towards high-performance lithium-ion batteries. Applied Surface Science, 2022, 580, 152319.	6.1	5
5	Robust Lithiumâ€“Sulfur Batteries Enabled by Highly Conductive WSe₂â€Based Superlattices with Tunable Interlayer Space. Advanced Functional Materials, 2022, 32, .	14.9	51
6	Enhanced Polysulfide Conversion with Highly Conductive and Electrocatalytic Iodineâ€Doped Bismuth Selenide Nanosheets in Lithiumâ€“Sulfur Batteries. Advanced Functional Materials, 2022, 32, .	14.9	49
7	Improved chloride binding stability for hydration products of calcium aluminates by phosphorus modification. Journal of the American Ceramic Society, 2022, 105, 4870-4882.	3.8	1
8	Calcium Poly(Heptazine Imide): A Covalent Heptazine Framework for Selective CO₂ Adsorption. ACS Nano, 2022, 16, 5393-5403.	14.6	17
9	Disrupting Sodium Ordering and Phase Transitions in a Layered Oxide Cathode. Journal of the Electrochemical Society, 2022, 169, 040504.	2.9	1
10	2D covalent organic frameworks for photosynthesis of Î±-trifluoromethylated ketones from aromatic alkenes. Applied Catalysis B: Environmental, 2022, 310, 121335.	20.2	41
11	Template-assisted synthesis of single-atom catalysts supported on highly crystalline vanadium pentoxide for stable oxygen evolution. Chem Catalysis, 2022, 2, 1191-1210.	6.1	8
12	Molybdenum Carbide Electrocatalyst In Situ Embedded in Porous Nitrogenâ€Rich Carbon Nanotubes Promotes Rapid Kinetics in Sodiumâ€Metalâ€“Sulfur Batteries. Advanced Materials, 2022, 34, e2106572.	21.0	33
13	H2O2 formation mechanisms on the (1 1 2) and (3 1 0) facets of SnO2 via water oxidation reaction with the participation of Bicarbonate: DFT and experimental Investigations. Applied Surface Science, 2022, 596, 153634.	6.1	4
14	Iterative redox activation promotes interfacial synergy in an Ag/CuxO catalyst for oxygen reduction. Chemical Engineering Journal, 2022, 446, 136966.	12.7	10
15	Atomically miniaturized bi-phase IrO_x/Ir catalysts loaded on N-doped carbon nanotubes for high-performance Liâ€“CO₂ batteries. Journal of Materials Chemistry A, 2022, 10, 19710-19721.	10.3	21
16	Atomistic Mechanisms of Binary Alloy Surface Segregation from Nanoseconds to Seconds Using Accelerated Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 4447-4455.	5.3	3
17	Phase Engineering of Defective Copper Selenide toward Robust Lithiumâ€“Sulfur Batteries. ACS Nano, 2022, 16, 11102-11114.	14.6	50
18	The role of antisite defect pairs in surface reconstruction of layered AMO2 oxides: A DFT+U study. Applied Surface Science, 2021, 537, 147750.	6.1	13

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19	One-Dimensional van der Waals Heterostructures as Efficient Metal-Free Oxygen Electrocatalysts. ACS Nano, 2021, 15, 3309-3319.	14.6	79
20	Electrochemical behavior of a Ni₃N OER precatalyst in Fe-purified alkaline media: the impact of self-oxidation and Fe incorporation. Materials Advances, 2021, 2, 2299-2309.	5.4	28
21	Stability of Pt Skin Intermetallic Core Catalysts and Adsorption Properties for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2021, 125, 3527-3534.	3.1	7
22	Liâ€“Zn Overlayer to Facilitate Uniform Lithium Deposition for Lithium Metal Batteries. ACS Applied Materials & Interfaces, 2021, 13, 9985-9993.	8.0	19
23	Unveiling the Role of Sulfur in Rapid Defluorination of Florfenicol by Sulfidized Nanoscale Zero-Valent Iron in Water under Ambient Conditions. Environmental Science & Technology, 2021, 55, 2628-2638.	10.0	98
24	3d Transitionâ€Metalâ€Mediated Columbite Nanocatalysts for Decentralized Electrosynthesis of Hydrogen Peroxide. Small, 2021, 17, e2007249.	10.0	35
25	Calculations of Hydrogen Associative Desorption on Mono- and Bimetallic Catalysts. Journal of Physical Chemistry C, 2021, 125, 12028-12037.	3.1	12
26	Factors that influence hydrogen binding at metal-atop sites. Journal of Chemical Physics, 2021, 155, 024703.	3.0	7
27	Multiscale vacancy and dislocation-mediated surface segregation in CuNi alloy up to microsecond timescales with accelerated dynamics. Microscopy and Microanalysis, 2021, 27, 2408-2410.	0.4	0
28	Low-Valent Metal Ions as MOF Pillars: A New Route Toward Stable and Multifunctional MOFs. Journal of the American Chemical Society, 2021, 143, 13710-13720.	13.7	43
29	Oxidation of Sn at the Clusterâ€“Support Interface: Sn and Ptâ€“Sn Clusters on TiO₂(110). Journal of Physical Chemistry C, 2021, 125, 17671-17683.	3.1	10
30	Rational Design of Coating Ions via Advantageous Surface Reconstruction in Highâ€Nickel Layered Oxide Cathodes for Lithiumâ€Ion Batteries. Advanced Energy Materials, 2021, 11, 2101112.	19.5	58
31	Controlling the Shape Anisotropy of Monoclinic Nb₁₂O₂₉ Nanocrystals Enables Tunable Electrochromic Spectral Range. Journal of the American Chemical Society, 2021, 143, 15745-15755.	13.7	23
32	Surfactant inhibition mechanisms of carbonate mineral dissolution in shale. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 625, 126857.	4.7	3
33	Coâ€“Feâ€“Cr (oxy)Hydroxides as Efficient Oxygen Evolution Reaction Catalysts. Advanced Energy Materials, 2021, 11, 2003412.	19.5	94
34	PTCDA Molecular Monolayer on Pb Thin Films: An Unusual <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math> -Electron Kondo System and Its Interplay with a Quantum-Confined Superconductor. Physical Review Letters, 2021, 127, 186805.	7.8	6
35	Black Tungsten Oxide Nanofiber as a Robust Support for Metal Catalysts: High Catalyst Loading for Electrochemical Oxygen Reduction. Small, 2021, 17, e2103755.	10.0	20
36	Outstanding Oxygen Reduction Reaction Catalytic Performance of Inâ€“PtNi Octahedral Nanoparticles Designed via Computational Dopant Screening. Chemistry of Materials, 2021, 33, 8895-8903.	6.7	17

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37	Correlating Surface Structures and Electrochemical Activity Using Shape-Controlled Single-Pt Nanoparticles. ACS Nano, 2021, 15, 17926-17937.	14.6	11
38	Solid State and Intercalation Chemistry of Nickel-Tellurate Cathodes for Lithium and Sodium Batteries. ECS Meeting Abstracts, 2021, MA2021-02, 204-204.	0.0	0
39	Atomic-Scale Mechanisms of Electrochemical Pt Dissolution. ACS Catalysis, 2021, 11, 14439-14447.	11.2	19
40	Tuning the Catalytic Preference of Ruthenium Catalysts for Nitrogen Reduction by Atomic Dispersion. Advanced Functional Materials, 2020, 30, 1905665.	14.9	159
41	Well-Defined Nanoparticle Electrocatalysts for the Refinement of Theory. Chemical Reviews, 2020, 120, 814-850.	47.7	75
42	Thiocyanate-Modified Silver Nanofoam for Efficient CO₂ Reduction to CO. ACS Catalysis, 2020, 10, 1444-1453.	11.2	51
43	Atomically Embedded Ag via Electrodiffusion Boosts Oxygen Evolution of CoOOH Nanosheet Arrays. ACS Catalysis, 2020, 10, 562-569.	11.2	93
44	Dechlorination and defluorination capability of sulfidized nanoscale zerovalent iron with suppressed water reactivity. Chemical Engineering Journal, 2020, 400, 125900.	12.7	61
45	Metal chalcogenide hollow polar bipyramid prisms as efficient sulfur hosts for Na-S batteries. Nature Communications, 2020, 11, 5242.	12.8	102
46	Octahedral Coordinated Trivalent Cobalt Enriched Multimetal Oxygenâ€Evolution Catalysts. Advanced Energy Materials, 2020, 10, 2002593.	19.5	47
47	Iron and Sulfur Precursors Affect Crystalline Structure, Speciation, and Reactivity of Sulfidized Nanoscale Zerovalent Iron. Environmental Science & Technology, 2020, 54, 13294-13303.	10.0	128
48	Amethyrin-type expanded porphyrins that display anti-aromatic character upon protonation. Chemical Communications, 2020, 56, 9994-9997.	4.1	13
49	Structural and Electrochemical Consequences of Sodium in the Transition-Metal Layer of Oâ€²3-Na₃Ni_{1.5}TeO₆. Chemistry of Materials, 2020, 32, 10035-10044.	6.7	14
50	Electrical and Structural Dual Function of Oxygen Vacancies for Promoting Electrochemical Capacitance in Tungsten Oxide. Small, 2020, 16, e2004709.	10.0	24
51	Embedded atom method potential for hydrogen on palladium surfaces. Journal of Molecular Modeling, 2020, 26, 336.	1.8	4
52	Synthesis and Dual-Mode Electrochromism of Anisotropic Monoclinic Nb₁₂O₂₉Colloidal Nanoplatelets. ACS Nano, 2020, 14, 10068-10082.	14.6	29
53	Au_xPd_(300â€x) Alloy Nanoparticles for the Oxygen Reduction Reaction in Alkaline Media. ChemElectroChem, 2020, 7, 3824-3831.	3.4	9
54	Surface Charge and Electrostatic Spin Crossover Effects in CoN₄ Electrocatalysts. ACS Catalysis, 2020, 10, 12148-12155.	11.2	69

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55	Insights into the multiple effects of oxygen vacancies on CuWO4 for photoelectrochemical water oxidation. Catalysis Science and Technology, 2020, 10, 7344-7351.	4.1	10
56	Evaluation of a V₈C₇ Anode for Oxygen Evolution in Alkaline Media: Unusual Morphological Behavior. ACS Sustainable Chemistry and Engineering, 2020, 8, 14101-14108.	6.7	6
57	Intrinsic Activity of Metal Centers in Metalâ€“Nitrogenâ€“Carbon Single-Atom Catalysts for Hydrogen Peroxide Synthesis. Journal of the American Chemical Society, 2020, 142, 21861-21871.	13.7	163
58	Identification of Active Sites of Pure and Nitrogen-Doped Carbon Materials for Oxygen Reduction Reaction Using Constant-Potential Calculations. Journal of Physical Chemistry C, 2020, 124, 12016-12023.	3.1	73
59	Catalytic activity atlas of ternary Coâ€“Feâ€“V metal oxides for the oxygen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 15951-15961.	10.3	43
60	Pair-distribution-function guided optimization of fingerprints for atom-centered neural network potentials. Journal of Chemical Physics, 2020, 152, 224102.	3.0	8
61	PdAg Alloy Nanocatalysts: Toward Economically Viable Nitrite Reduction in Drinking Water. ACS Catalysis, 2020, 10, 7979-7989.	11.2	64
62	Cu_xIr_{1â€“x} Nanoalloy Catalysts Achieve Near 100% Selectivity for Aqueous Nitrite Reduction to NH₃. ACS Catalysis, 2020, 10, 7915-7921.	11.2	69
63	Calculations of selective Si epitaxial growth. Applied Surface Science, 2020, 514, 145888.	6.1	2
64	Reversible Solid-State Isomerism of Azobenzene-Loaded Large-Pore Isoreticular Mg-CUK-1. Journal of the American Chemical Society, 2020, 142, 6467-6471.	13.7	18
65	Cobalt Metalâ€“Cobalt Carbide Composite Microspheres for Water Reduction Electrocatalysis. ACS Applied Energy Materials, 2020, 3, 3909-3918.	5.1	32
66	Sulfur Loading and Speciation Control the Hydrophobicity, Electron Transfer, Reactivity, and Selectivity of Sulfidized Nanoscale Zerovalent Iron. Advanced Materials, 2020, 32, e1906910.	21.0	204
67	Hydrogen desorption from the surface and subsurface of cobalt. Physical Chemistry Chemical Physics, 2020, 22, 15281-15287.	2.8	7
68	Highly reversible oxygen redox in layered compounds enabled by surface polyanions. Nature Communications, 2020, 11, 3411.	12.8	54
69	Reviving reversible anion redox in 3d-transition-metal Li rich oxides by introducing surface defects. Nano Energy, 2020, 71, 104644.	16.0	31
70	Intermetallic Pd₃Pb nanocubes with high selectivity for the 4-electron oxygen reduction reaction pathway. Nanoscale, 2020, 12, 2532-2541.	5.6	33
71	Effect of TiO_x Substrate Interactions on the Electrocatalytic Oxygen Reduction Reaction at Au Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 10045-10056.	3.1	14
72	Testing the predictive power of theory for Pd_xIr_(100â^'x) alloy nanoparticles for the oxygen reduction reaction. Journal of Materials Chemistry A, 2020, 8, 8421-8429.	10.3	9

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73	Bioinspired CNP Iron(II) Pincers Relevant to [Fe]-Hydrogenase (Hmd): Effect of Dicarbonyl versus Monocarbonyl Motifs in H₂ Activation and Transfer Hydrogenation. Inorganic Chemistry, 2020, 59, 2548-2561.	4.0	2
74	Low temperature dissociation of CO on manganese promoted cobalt(poly). Chemical Communications, 2020, 56, 2865-2868.	4.1	2
75	Off-Lattice Kinetic Monte Carlo Methods. , 2020, , 715-743.		5
76	Design of a Pdâ€“Au Nitrite Reduction Catalyst by Identifying and Optimizing Active Ensembles. ACS Catalysis, 2019, 9, 7957-7966.	11.2	160
77	Vanadium(III) Acetylacetonate as an Efficient Soluble Catalyst for Lithiumâ€“Oxygen Batteries. Angewandte Chemie, 2019, 131, 12683-12687.	2.0	22
78	Vanadium(III) Acetylacetonate as an Efficient Soluble Catalyst for Lithiumâ€“Oxygen Batteries. Angewandte Chemie - International Edition, 2019, 58, 12553-12557.	13.8	53
79	Electrochemical Properties of Three Li₂Ni₂TeO₆ Structural Polymorphs. Chemistry of Materials, 2019, 31, 9379-9388.	6.7	29
80	Rational Design of Rhodiumâ€“Iridium Alloy Nanoparticles as Highly Active Catalysts for Acidic Oxygen Evolution. ACS Nano, 2019, 13, 13225-13234.	14.6	151
81	Cu₄SnS₄-Rich Nanomaterials for Thin-Film Lithium Batteries with Enhanced Conversion Reaction. ACS Nano, 2019, 13, 10671-10681.	14.6	26
82	Ionic and Electronic Conduction in TiNb₂O₇. Journal of the American Chemical Society, 2019, 141, 16706-16725.	13.7	134
83	Solving the Structure and Dynamics of Metal Nanoparticles by Combining X-Ray Absorption Fine Structure Spectroscopy and Atomistic Structure Simulations. Annual Review of Analytical Chemistry, 2019, 12, 501-522.	5.4	27
84	Off-Lattice Kinetic Monte Carlo Methods. , 2019, , 1-29.		3
85	Theoretical Resolution of the Exceptional Oxygen Reduction Activity of Au(100) in Alkaline Media. ACS Catalysis, 2019, 9, 5567-5573.	11.2	93
86	Selectivity for ethanol partial oxidation: the unique chemistry of single-atom alloy catalysts on Au, Ag, and Cu(111). Journal of Materials Chemistry A, 2019, 7, 23868-23877.	10.3	80
87	Adaptive kinetic Monte Carlo simulations of surface segregation in PdAu nanoparticles. Nanoscale, 2019, 11, 10524-10535.	5.6	25
88	Alkali Atoms Diffusion Mechanism in CuInSe₂ Explained by Kinetic Monte Carlo Simulations. Advanced Theory and Simulations, 2019, 2, 1900036.	2.8	12
89	Oxidative Cross-Esterification and Related Pathways of Co-Adsorbed Oxygen and Ethanol on Pdâ€“Au. ACS Catalysis, 2019, 9, 4516-4525.	11.2	28
90	Selective Oxidation of Acetaldehyde to Acetic Acid on Pdâ€“Au Bimetallic Model Catalysts. ACS Catalysis, 2019, 9, 4360-4368.	11.2	26

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91	Computational design of CO-tolerant Pt₃M anode electrocatalysts for proton-exchange membrane fuel cells. Physical Chemistry Chemical Physics, 2019, 21, 4046-4052.	2.8	14
92	Big to Small: Ultrafine Mo₂C Particles Derived from Giant Polyoxomolybdate Clusters for Hydrogen Evolution Reaction. Small, 2019, 15, e1900358.	10.0	53
93	Stabilizer-Free CuIr Alloy Nanoparticle Catalysts. Chemistry of Materials, 2019, 31, 10225-10235.	6.7	16
94	Theory-guided design of catalytic materials using scaling relationships and reactivity descriptors. Nature Reviews Materials, 2019, 4, 792-804.	48.7	338
95	Combined Experimental and Theoretical Study of the Structure of AuPt Nanoparticles Prepared by Galvanic Exchange. Langmuir, 2019, 35, 16496-16507.	3.5	1
96	Enhanced Activity Promoted by CeO_x on a CoO_x Electrocatalyst for the Oxygen Evolution Reaction. ACS Catalysis, 2018, 8, 4257-4265.	11.2	151
97	Honeycombâ€Like Spherical Cathode Host Constructed from Hollow Metallic and Polar Co₉S₈ Tubules for Advanced Lithiumâ€“Sulfur Batteries. Advanced Functional Materials, 2018, 28, 1704443.	14.9	236
98	A computational study of supported Cu-based bimetallic nanoclusters for CO oxidation. Physical Chemistry Chemical Physics, 2018, 20, 7508-7513.	2.8	17
99	Kinetic Monte Carlo Study of Li Intercalation in LiFePO₄. ACS Nano, 2018, 12, 844-851.	14.6	47
100	Oxygen Reduction Reaction on Classically Immiscible Bimetallics: A Case Study of RhAu. Journal of Physical Chemistry C, 2018, 122, 2712-2716.	3.1	123
101	New Mechanism for Ferroelectricity in the Perovskite Ca_{2â€“x}Mn_xTi₂O₆ Synthesized by Spark Plasma Sintering. Journal of the American Chemical Society, 2018, 140, 2214-2220.	13.7	32
102	Calculations of CO Oxidation over a Au/TiO₂ Catalyst: A Study of Active Sites, Catalyst Deactivation, and Moisture Effects. ACS Catalysis, 2018, 8, 1376-1383.	11.2	64
103	Rapid Synthesis of Rhodiumâ€“Palladium Alloy Nanocatalysts. ChemCatChem, 2018, 10, 329-333.	3.7	19
104	Superior Oxygen Electrocatalysis on RuSe x Nanoparticles for Rechargeable Air Cathodes. Advanced Energy Materials, 2018, 8, 1702037.	19.5	13
105	A highly efficient double-hierarchical sulfur host for advanced lithiumâ€“sulfur batteries. Chemical Science, 2018, 9, 666-675.	7.4	97
106	Probing Dynamic Processes of the Initial Stages of Cu(100) Surface Oxidation by in situ Environmental TEM and Multiscale Simulations. Microscopy and Microanalysis, 2018, 24, 262-263.	0.4	4
107	Off-Lattice Kinetic Monte Carlo Methods. , 2018, , 1-29.		0
108	Structural characterization of heterogeneous RhAu nanoparticles from a microwave-assisted synthesis. Nanoscale, 2018, 10, 22520-22532.	5.6	15

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109	Calculations of the pH-Dependent Onset Potential for CO Electrooxidation on Au(111). Langmuir, 2018, 34, 15268-15275.	3.5	18
110	Effects of ensembles, ligand, and strain on adsorbate binding to alloy surfaces. Journal of Chemical Physics, 2018, 149, 174705.	3.0	193
111	Na₃MnZr(PO₄)₃: A High-Voltage Cathode for Sodium Batteries. Journal of the American Chemical Society, 2018, 140, 18192-18199.	13.7	195
112	Microwave-Assisted Synthesis of Classically Immiscible Agâ€“Ir Alloy Nanoparticle Catalysts. ACS Catalysis, 2018, 8, 11386-11397.	11.2	57
113	Electrocatalytic Study of the Oxygen Reduction Reaction at Gold Nanoparticles in the Absence and Presence of Interactions with SnO_x Supports. Journal of the American Chemical Society, 2018, 140, 13775-13785.	13.7	42
114	Ethanol Decomposition on Pdâ€“Au Alloy Catalysts. Journal of Physical Chemistry C, 2018, 122, 22024-22032.	3.1	77
115	Chinese knot-like electrode design for advanced Li-S batteries. Nano Energy, 2018, 53, 354-361.	16.0	72
116	Formation of HONO from the NH₃-promoted hydrolysis of NO₂dimers in the atmosphere. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 7236-7241.	7.1	67
117	Chloride Flux Growth of Idiomorphic AWO₄ (A = Sr, Ba) Single Microcrystals. Crystal Growth and Design, 2018, 18, 5301-5310.	3.0	8
118	Experimental and Theoretical Structural Investigation of AuPt Nanoparticles Synthesized Using a Direct Electrochemical Method. Journal of the American Chemical Society, 2018, 140, 6249-6259.	13.7	33
119	A Metalâ€“Organic Framework with Cooperative Phosphines That Permit Postâ€Synthetic Installation of Open Metal Sites. Angewandte Chemie, 2018, 130, 9439-9443.	2.0	13
120	A Metalâ€“Organic Framework with Cooperative Phosphines That Permit Postâ€Synthetic Installation of Open Metal Sites. Angewandte Chemie - International Edition, 2018, 57, 9295-9299.	13.8	52
121	Synergistic Coupling of Metallic Cobalt Nitride Nanofibers and IrO_x Nanoparticle Catalysts for Stable Oxygen Evolution. Chemistry of Materials, 2018, 30, 5941-5950.	6.7	57
122	The effect of single pd atoms on the energetics of recombinative O2 desorption from Au(111). Surface Science, 2018, 677, 296-300.	1.9	20
123	Calculations of Oxygen Adsorption-Induced Surface Reconstruction and Oxide Formation on Cu(100). Chemistry of Materials, 2017, 29, 1472-1484.	6.7	12
124	Atomistic Simulations of Activated Processes in Materials. Annual Review of Materials Research, 2017, 47, 199-216.	9.3	38
125	Interface engineering for a rational design of poison-free bimetallic CO oxidation catalysts. Nanoscale, 2017, 9, 5244-5253.	5.6	28
126	PdAu Alloy Nanoparticle Catalysts: Effective Candidates for Nitrite Reduction in Water. ACS Catalysis, 2017, 7, 3268-3276.	11.2	89

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127	Communication: Calculations of the (2 Ã— 1)-O reconstruction kinetics on Cu(110). Journal of Chemical Physics, 2017, 146, 111101.	3.0	8
128	Tunability of the Adsorbate Binding on Bimetallic Alloy Nanoparticles for the Optimization of Catalytic Hydrogenation. Journal of the American Chemical Society, 2017, 139, 5538-5546.	13.7	96
129	Mechanistic insights on ethanol dehydrogenation on Pdâ€“Au model catalysts: a combined experimental and DFT study. Physical Chemistry Chemical Physics, 2017, 19, 30578-30589.	2.8	57
130	Self-Assembled Cuâ€“Snâ€“S Nanotubes with High (De)Lithiation Performance. ACS Nano, 2017, 11, 10347-10356.	14.6	35
131	Understanding the phase transitions in spinel-layered-rock salt system: Criterion for the rational design of LLO/spinel nanocomposites. Nano Energy, 2017, 40, 566-575.	16.0	58
132	Characterization of hydrogen bonding motifs in proteins: hydrogen elimination monitoring by ultraviolet photodissociation mass spectrometry. Physical Chemistry Chemical Physics, 2017, 19, 20057-20074.	2.8	12
133	Transformation of topologically close-packed Î²-W to body-centered cubic Î±-W: Comparison of experiments and computations. Journal of Chemical Physics, 2017, 147, 152709.	3.0	22
134	Detection of CO₂^{â€¢â€“} in the Electrochemical Reduction of Carbon Dioxide in N,N-Dimethylformamide by Scanning Electrochemical Microscopy. Journal of the American Chemical Society, 2017, 139, 18552-18557.	13.7	84
135	Computationally Assisted STEM and EXAFS Characterization of Tunable Rh/Au and Rh/Ag Bimetallic Nanoparticle Catalysts. Microscopy and Microanalysis, 2017, 23, 2030-2031.	0.4	10
136	Dehydrogenation Selectivity of Ethanol on Close-Packed Transition Metal Surfaces: A Computational Study of Monometallic, Pd/Au, and Rh/Au Catalysts. Journal of Physical Chemistry C, 2017, 121, 27504-27510.	3.1	96
137	Oxygen activity and peroxide formation as charge compensation mechanisms in Li₂MnO₃. Journal of Materials Chemistry A, 2017, 5, 15183-15190.	10.3	55
138	Structural transformations in Li₂MnSiO₄: evidence that a Li intercalation material can reversibly cycle through a disordered phase. Journal of Materials Chemistry A, 2017, 5, 16722-16731.	10.3	22
139	Preface: Special Topic on Reaction Pathways. Journal of Chemical Physics, 2017, 147, 152401.	3.0	1
140	Breaking Down the Crystallinity: The Path for Advanced Lithium Batteries. Advanced Energy Materials, 2016, 6, 1501933.	19.5	77
141	Calculations of oxide formation on low-index Cu surfaces. Journal of Chemical Physics, 2016, 145, 044711.	3.0	25
142	Localized Mg-vacancy states in the thermoelectric material Mg2â^'Î´Si0.4Sn0.6. Journal of Applied Physics, 2016, 119, .	2.5	9
143	Computational screening of core@shell nanoparticles for the hydrogen evolution and oxygen reduction reactions. Journal of Chemical Physics, 2016, 145, 244708.	3.0	22
144	A combined theoretical and experimental EXAFS study of the structure and dynamics of Au₁₄₇ nanoparticles. Catalysis Science and Technology, 2016, 6, 6879-6885.	4.1	26

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145	Efficient CO Oxidation Using Dendrimer-Encapsulated Pt Nanoparticles Activated with <2% Cu Surface Atoms. ACS Nano, 2016, 10, 8760-8769.	14.6	39
146	Linear topology in amorphous metal oxide electrochromic networks obtained via low-temperature solution processing. Nature Materials, 2016, 15, 1267-1273.	27.5	155
147	Improved Charge Carrier Transport of Hydrogen-Treated Copper Tungstate: Photoelectrochemical and Computational Study. Journal of the Electrochemical Society, 2016, 163, H970-H975.	2.9	17
148	Can Exciton-Delocalizing Ligands Facilitate Hot Hole Transfer from Semiconductor Nanocrystals?. Journal of Physical Chemistry C, 2016, 120, 28224-28234.	3.1	20
149	Simple Synthesis of Nanocrystalline Tin Sulfide/N-Doped Reduced Graphene Oxide Composites as Lithium Ion Battery Anodes. ACS Nano, 2016, 10, 10778-10788.	14.6	178
150	Anomalous bulk modulus in vanadate spinels. Physical Review B, 2016, 94, .	3.2	9
151	H-bonding of an NH3 gas molecule to H2O/Pt(111) â€" A barrier-free path. Journal of Chemical Physics, 2016, 144, 054701.	3.0	3
152	Ethylene binding to Au/Cu alloy nanoparticles. Surface Science, 2016, 653, 66-70.	1.9	8
153	Microwave-Assisted Synthesis of Pd_xAu_{100â€“x} Alloy Nanoparticles: A Combined Experimental and Theoretical Assessment of Synthetic and Compositional Effects upon Catalytic Reactivity. ACS Catalysis, 2016, 6, 4882-4893.	11.2	54
154	Engineering the Mechanical Properties of Monolayer Graphene Oxide at the Atomic Level. Journal of Physical Chemistry Letters, 2016, 7, 2702-2707.	4.6	60
155	Collective Atomic Displacements during Complex Phase Boundary Migration in Solid-Solid Phase Transformations. Physical Review Letters, 2016, 116, 035701.	7.8	17
156	Analytic dynamical corrections to transition state theory. New Journal of Physics, 2016, 18, 013023.	2.9	22
157	O₂ activation at the Au/MgO(001) interface boundary facilitates CO oxidation. Physical Chemistry Chemical Physics, 2016, 18, 5486-5490.	2.8	13
158	Computational Design of a CeO₂-Supported Pd-Based Bimetallic Nanorod for CO Oxidation. Journal of Physical Chemistry C, 2016, 120, 5557-5564.	3.1	42
159	Distributed replica dynamics. Journal of Chemical Physics, 2015, 143, 174112.	3.0	1
160	Ridge-based bias potentials to accelerate molecular dynamics. Journal of Chemical Physics, 2015, 143, 244104.	3.0	7
161	Electrochemical Activity of Dendrimer-Stabilized Tin Nanoparticles for Lithium Alloying Reactions. Langmuir, 2015, 31, 6570-6576.	3.5	10
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