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 climbing image nudged elastic band method for finding saddle points and minimum energy paths. Journal of Chemical Physics, 2000, 113, 9901-9904.	3.0	15,067
2	A fast and robust algorithm for Bader decomposition of charge density. Computational Materials Science, 2006, 36, 354-360.	3.0	7,727
3	Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points. Journal of Chemical Physics, 2000, 113, 9978-9985.	3.0	7,115
4	A grid-based Bader analysis algorithm without lattice bias. Journal of Physics Condensed Matter, 2009, 21, 084204.	1.8	4,245
5	Improved grid-based algorithm for Bader charge allocation. Journal of Computational Chemistry, 2007, 28, 899-908.	3.3	3,175
6	A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives. Journal of Chemical Physics, 1999, 111, 7010-7022.	3.0	2,505
7	Optimization methods for finding minimum energy paths. Journal of Chemical Physics, 2008, 128, 134106.	3.0	1,360
8	A generalized solid-state nudged elastic band method. Journal of Chemical Physics, 2012, 136, 074103.	3.0	701
9	Removal of Interstitial H₂O in Hexacyanometallates for a Superior Cathode of a Sodium-Ion Battery. Journal of the American Chemical Society, 2015, 137, 2658-2664.	13.7	654
10	CO Oxidation Mechanism on CeO₂-Supported Au Nanoparticles. Journal of the American Chemical Society, 2012, 134, 1560-1570.	13.7	496
11	Comparison of methods for finding saddle points without knowledge of the final states. Journal of Chemical Physics, 2004, 121, 9776-9792.	3.0	462
12	Long time scale kinetic Monte Carlo simulations without lattice approximation and predefined event table. Journal of Chemical Physics, 2001, 115, 9657-9666.	3.0	398
13	Lithium Insertion in Nanostructured TiO₂(B) Architectures. Accounts of Chemical Research, 2013, 46, 1104-1112.	15.6	393
14	A Systematic Investigation of p-Nitrophenol Reduction by Bimetallic Dendrimer Encapsulated Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 7598-7604.	3.1	349
15	Theory-guided design of catalytic materials using scaling relationships and reactivity descriptors. Nature Reviews Materials, 2019, 4, 792-804.	48.7	338
16	Calculations of Li-Ion Diffusion in Olivine Phosphates. Chemistry of Materials, 2011, 23, 4032-4037.	6.7	249
17	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
18	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

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19	Na₃MnZr(PO₄)₃: A High-Voltage Cathode for Sodium Batteries. Journal of the American Chemical Society, 2018, 140, 18192-18199.	13.7	195
20	Effects of ensembles, ligand, and strain on adsorbate binding to alloy surfaces. Journal of Chemical Physics, 2018, 149, 174705.	3.0	193
21	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
22	Water-Enhanced Low-Temperature CO Oxidation and Isotope Effects on Atomic Oxygen-Covered Au(111). Journal of the American Chemical Society, 2008, 130, 6801-6812.	13.7	171
23	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
24	Paths to which the nudged elastic band converges. Journal of Computational Chemistry, 2011, 32, 1769-1771.	3.3	162
25	Design of a Pdâ€“Au Nitrite Reduction Catalyst by Identifying and Optimizing Active Ensembles. ACS Catalysis, 2019, 9, 7957-7966.	11.2	160
26	Tuning the Catalytic Preference of Ruthenium Catalysts for Nitrogen Reduction by Atomic Dispersion. Advanced Functional Materials, 2020, 30, 1905665.	14.9	159
27	Theoretical calculations of CH4 and H2 associative desorption from Ni(111): Could subsurface hydrogen play an important role?. Journal of Chemical Physics, 2006, 124, 044706.	3.0	156
28	Linear topology in amorphous metal oxide electrochromic networks obtained via low-temperature solution processing. Nature Materials, 2016, 15, 1267-1273.	27.5	155
29	Hybrid density functional theory band structure engineering in hematite. Journal of Chemical Physics, 2011, 134, 224706.	3.0	152
30	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
31	Rational Design of Rhodiumâ€“Iridium Alloy Nanoparticles as Highly Active Catalysts for Acidic Oxygen Evolution. ACS Nano, 2019, 13, 13225-13234.	14.6	151
32	CO Oxidation at the Interface of Au Nanoclusters and the Stepped-CeO₂(111) Surface by the Marsâ€“van Krevelen Mechanism. Journal of Physical Chemistry Letters, 2013, 4, 216-221.	4.6	148
33	Charge redistribution in core-shell nanoparticles to promote oxygen reduction. Journal of Chemical Physics, 2009, 130, 194504.	3.0	141
34	Design of Pt-Shell Nanoparticles with Alloy Cores for the Oxygen Reduction Reaction. ACS Nano, 2013, 7, 9168-9172.	14.6	141
35	Theoretical Calculations of Dissociative Adsorption ofCH4on an Ir(111) Surface. Physical Review Letters, 2001, 86, 664-667.	7.8	136
36	Ionic and Electronic Conduction in TiNb₂O₇. Journal of the American Chemical Society, 2019, 141, 16706-16725.	13.7	134

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37	Methods for Finding Saddle Points and Minimum Energy Paths. , 2002, , 269-302.		133
38	Catalytic Activity of Pd/Cu Random Alloy Nanoparticles for Oxygen Reduction. Journal of Physical Chemistry Letters, 2011, 2, 1328-1331.	4.6	131
39	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
40	Adaptive kinetic Monte Carlo for first-principles accelerated dynamics. Journal of Chemical Physics, 2008, 129, 114104.	3.0	125
41	Intrinsic Diffusion of Hydrogen on Rutile TiO₂(110). Journal of the American Chemical Society, 2008, 130, 9080-9088.	13.7	124
42	Oxygen Reduction Reaction on Classically Immiscible Bimetallics: A Case Study of RhAu. Journal of Physical Chemistry C, 2018, 122, 2712-2716.	3.1	123
43	Microwave Synthesis of Classically Immiscible Rhodiumâ€“Silver and Rhodiumâ€“Gold Alloy Nanoparticles: Highly Active Hydrogenation Catalysts. ACS Nano, 2014, 8, 11512-11521.	14.6	118
44	Solid-state dimer method for calculating solid-solid phase transitions. Journal of Chemical Physics, 2014, 140, 174104.	3.0	112
45	Interfacial adhesion between graphene and silicon dioxide by density functional theory with van der Waals corrections. Journal Physics D: Applied Physics, 2014, 47, 255301.	2.8	109
46	Potential Energy Surface of Methanol Decomposition on Cu(110). Journal of Physical Chemistry C, 2009, 113, 4522-4537.	3.1	105
47	Calculations of Oxygen Stability in Lithium-Rich Layered Cathodes. Journal of Physical Chemistry C, 2012, 116, 23201-23204.	3.1	104
48	Efficient Electrocatalytic Oxidation of Formic Acid Using Au@Pt Dendrimer-Encapsulated Nanoparticles. Journal of the American Chemical Society, 2013, 135, 5521-5524.	13.7	103
49	CO Oxidation at the Interface between Doped CeO₂ and Supported Au Nanoclusters. Journal of Physical Chemistry Letters, 2012, 3, 2194-2199.	4.6	102
50	Metal chalcogenide hollow polar bipyramid prisms as efficient sulfur hosts for Na-S batteries. Nature Communications, 2020, 11, 5242.	12.8	102
51	CO Oxidation at the Au/TiO₂ Boundary: The Role of the Au/Ti_{5c} Site. ACS Catalysis, 2015, 5, 1589-1595.	11.2	99
52	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
53	A highly efficient double-hierarchical sulfur host for advanced lithiumâ€“sulfur batteries. Chemical Science, 2018, 9, 666-675.	7.4	97
54	Structure and Mobility of Defects Formed from Collision Cascades in MgO. Physical Review Letters, 2004, 92, 115505.	7.8	96

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55	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
56	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
57	Theoretical Study of the Structural Evolution of a Na₂FeMn(CN)₆ Cathode upon Na Intercalation. Chemistry of Materials, 2015, 27, 3763-3768.	6.7	94
58	Coâ€“Feâ€“Cr (oxy)Hydroxides as Efficient Oxygen Evolution Reaction Catalysts. Advanced Energy Materials, 2021, 11, 2003412.	19.5	94
59	Theoretical Resolution of the Exceptional Oxygen Reduction Activity of Au(100) in Alkaline Media. ACS Catalysis, 2019, 9, 5567-5573.	11.2	93
60	Atomically Embedded Ag via Electrodiffusion Boosts Oxygen Evolution of CoOOH Nanosheet Arrays. ACS Catalysis, 2020, 10, 562-569.	11.2	93
61	Optimizing transition states via kernel-based machine learning. Journal of Chemical Physics, 2012, 136, 174101.	3.0	92
62	Theoretical and Experimental Study of Vanadium-Based Fluorophosphate Cathodes for Rechargeable Batteries. Chemistry of Materials, 2014, 26, 3089-3097.	6.7	90
63	Model studies of heterogeneous catalytic hydrogenation reactions with gold. Chemical Society Reviews, 2013, 42, 5002.	38.1	89
64	PdAu Alloy Nanoparticle Catalysts: Effective Candidates for Nitrite Reduction in Water. ACS Catalysis, 2017, 7, 3268-3276.	11.2	89
65	Small Pd Clusters, up to the Tetramer At Least, Are Highly Mobile on the MgO(100) Surface. Physical Review Letters, 2005, 95, 146103.	7.8	87
66	Morphological Dependence of Lithium Insertion in Nanocrystalline TiO₂(B) Nanoparticles and Nanosheets. Journal of Physical Chemistry Letters, 2012, 3, 2015-2019.	4.6	87
67	Multiple Time Scale Simulations of Metal Crystal Growth Reveal the Importance of Multiatom Surface Processes. Physical Review Letters, 2003, 90, 116101.	7.8	86
68	Understanding the Nucleation and Growth of Metals on TiO₂: Co Compared to Au, Ni, and Pt. Journal of Physical Chemistry C, 2013, 117, 7191-7201.	3.1	84
69	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
70	CO Adsorption-Driven Surface Segregation of Pd on Au/Pd Bimetallic Surfaces: Role of Defects and Effect on CO Oxidation. ACS Catalysis, 2013, 3, 2541-2546.	11.2	83
71	CO Oxidation at the Auâ€“Cu Interface of Bimetallic Nanoclusters Supported on CeO₂(111). Journal of Physical Chemistry Letters, 2013, 4, 2943-2947.	4.6	80
72	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

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73	Dynamical simulations of radiation damage and defect mobility in MgO. Physical Review B, 2005, 71, .	3.2	79
74	One-Dimensional van der Waals Heterostructures as Efficient Metal-Free Oxygen Electrocatalysts. ACS Nano, 2021, 15, 3309-3319.	14.6	79
75	A Theoretical and Experimental Approach for Correlating Nanoparticle Structure and Electrocatalytic Activity. Accounts of Chemical Research, 2015, 48, 1351-1357.	15.6	78
76	Breaking Down the Crystallinity: The Path for Advanced Lithium Batteries. Advanced Energy Materials, 2016, 6, 1501933.	19.5	77
77	Ethanol Decomposition on Pdâ€“Au Alloy Catalysts. Journal of Physical Chemistry C, 2018, 122, 22024-22032.	3.1	77
78	An Experimental and Theoretical Investigation of the Inversion of Pd@Pt Core@Shell Dendrimer-Encapsulated Nanoparticles. ACS Nano, 2013, 7, 9345-9353.	14.6	75
79	Well-Defined Nanoparticle Electrocatalysts for the Refinement of Theory. Chemical Reviews, 2020, 120, 814-850.	47.7	75
80	Characterization and Theory of Electrocatalysts Based on Scanning Electrochemical Microscopy Screening Methods. Langmuir, 2006, 22, 10426-10431.	3.5	74
81	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
82	Chinese knot-like electrode design for advanced Li-S batteries. Nano Energy, 2018, 53, 354-361.	16.0	72
83	Periodicity and Atomic Ordering in Nanosized Particles of Crystals. Journal of Physical Chemistry C, 2008, 112, 8907-8911.	3.1	70
84	First principles study of photo-oxidation degradation mechanisms in P3HT for organic solar cells. Physical Chemistry Chemical Physics, 2014, 16, 8092-8099.	2.8	70
85	In situ Raman spectroscopy of LiFePO₄: size and morphology dependence during charge and self-discharge. Nanotechnology, 2013, 24, 424009.	2.6	69
86	Surface Charge and Electrostatic Spin Crossover Effects in CoN₄ Electrocatalysts. ACS Catalysis, 2020, 10, 12148-12155.	11.2	69
87	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
88	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
89	Pd diffusion on MgO(100): The role of defects and small cluster mobility. Surface Science, 2006, 600, 1351-1362.	1.9	66
90	Optimizing core-shell nanoparticle catalysts with a genetic algorithm. Journal of Chemical Physics, 2009, 131, 234103.	3.0	66

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91	MgO addimer diffusion on MgO(100): A comparison ofab initioand empirical models. Physical Review B, 2005, 72, .	3.2	64
92	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
93	PdAg Alloy Nanocatalysts: Toward Economically Viable Nitrite Reduction in Drinking Water. ACS Catalysis, 2020, 10, 7979-7989.	11.2	64
94	A theoretical and experimental examination of systematic ligand-induced disorder in Au dendrimer-encapsulated nanoparticles. Chemical Science, 2013, 4, 2912.	7.4	63
95	Enhanced Charge-Transfer Kinetics by Anion Surface Modification of LiFePO₄. Chemistry of Materials, 2012, 24, 3212-3218.	6.7	62
96	Unification of algorithms for minimum mode optimization. Journal of Chemical Physics, 2014, 140, 044115.	3.0	62
97	CO Oxidation on the Pd(111) Surface. ACS Catalysis, 2014, 4, 3435-3443.	11.2	62
98	Dechlorination and defluorination capability of sulfidized nanoscale zerovalent iron with suppressed water reactivity. Chemical Engineering Journal, 2020, 400, 125900.	12.7	61
99	Engineering the Mechanical Properties of Monolayer Graphene Oxide at the Atomic Level. Journal of Physical Chemistry Letters, 2016, 7, 2702-2707.	4.6	60
100	Adaptive kinetic Monte Carlo simulation of methanol decomposition on Cu(100). Journal of Chemical Physics, 2009, 131, 244520.	3.0	59
101	Mechanism for the waterâ€“gas shift reaction on monofunctional platinum and cause of catalyst deactivation. Journal of Catalysis, 2011, 282, 278-288.	6.2	58
102	Tuning the Oxygen Reduction Activity of Pd Shell Nanoparticles with Random Alloy Cores. Journal of Physical Chemistry C, 2012, 116, 20860-20865.	3.1	58
103	Sodium Intercalation Behavior of Layered Na_xNbS₂ (0 â‰¤ x â‰¤ 1). Chemistry of Materials, 2013, 25, 1699-1705.	6.7	58
104	EON: software for long time simulations of atomic scale systems. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 055002.	2.0	58
105	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
106	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
107	Alchemical derivatives of reaction energetics. Journal of Chemical Physics, 2010, 133, 084104.	3.0	57
108	Oxygen Activation and Reaction on Pdâ€“Au Bimetallic Surfaces. Journal of Physical Chemistry C, 2015, 119, 11754-11762.	3.1	57

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109	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
110	Microwave-Assisted Synthesis of Classically Immiscible Agâ€“Ir Alloy Nanoparticle Catalysts. ACS Catalysis, 2018, 8, 11386-11397.	11.2	57
111	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
112	Au@Pt dendrimer encapsulated nanoparticles as model electrocatalysts for comparison of experiment and theory. Chemical Science, 2012, 3, 1033.	7.4	56
113	Oxygen activity and peroxide formation as charge compensation mechanisms in Li₂MnO₃. Journal of Materials Chemistry A, 2017, 5, 15183-15190.	10.3	55
114	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
115	Highly reversible oxygen redox in layered compounds enabled by surface polyanions. Nature Communications, 2020, 11, 3411.	12.8	54
116	Vanadium(III) Acetylacetonate as an Efficient Soluble Catalyst for Lithiumâ€“Oxygen Batteries. Angewandte Chemie - International Edition, 2019, 58, 12553-12557.	13.8	53
117	Big to Small: Ultrafine Mo₂C Particles Derived from Giant Polyoxomolybdate Clusters for Hydrogen Evolution Reaction. Small, 2019, 15, e1900358.	10.0	53
118	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
119	Dimer saddle point searches to determine the reactivity of formate on Cu(111). Journal of Catalysis, 2008, 258, 44-51.	6.2	51
120	Suppressing the bipolar contribution to the thermoelectric properties of Mg2Si0.4Sn0.6 by Ge substitution. Journal of Applied Physics, 2015, 117, .	2.5	51
121	Thiocyanate-Modified Silver Nanofoam for Efficient CO₂ Reduction to CO. ACS Catalysis, 2020, 10, 1444-1453.	11.2	51
122	Robust Lithiumâ€“Sulfur Batteries Enabled by Highly Conductive WSe₂â€Based Superlattices with Tunable Interlayer Space. Advanced Functional Materials, 2022, 32, .	14.9	51
123	Phase Engineering of Defective Copper Selenide toward Robust Lithiumâ€“Sulfur Batteries. ACS Nano, 2022, 16, 11102-11114.	14.6	50
124	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
125	Kinetic Monte Carlo Study of Li Intercalation in LiFePO₄. ACS Nano, 2018, 12, 844-851.	14.6	47
126	Octahedral Coordinated Trivalent Cobalt Enriched Multimetal Oxygenâ€Evolution Catalysts. Advanced Energy Materials, 2020, 10, 2002593.	19.5	47

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127	Calcium Adsorption on MgO(100):â€‰ Energetics, Structure, and Role of Defects. Journal of the American Chemical Society, 2008, 130, 2314-2322.	13.7	45
128	Site-Selective Cu Deposition on Pt Dendrimer-Encapsulated Nanoparticles: Correlation of Theory and Experiment. Journal of the American Chemical Society, 2012, 134, 4153-4162.	13.7	44
129	Benchmarks for Characterization of Minima, Transition States, and Pathways in Atomic, Molecular, and Condensed Matter Systems. Journal of Chemical Theory and Computation, 2014, 10, 5476-5482.	5.3	43
130	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
131	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
132	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
133	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
134	Kinetic and Thermodynamic Evaluation of the Reversible N-Heterocyclic Carbeneâ^'Isothiocyanate Coupling Reaction: Applications in Latent Catalysis. Journal of Organic Chemistry, 2011, 76, 301-304.	3.2	41
135	2D covalent organic frameworks for photosynthesis of Î±-trifluoromethylated ketones from aromatic alkenes. Applied Catalysis B: Environmental, 2022, 310, 121335.	20.2	41
136	Probing the Limits of Conventional Extended X-ray Absorption Fine Structure Analysis Using Thiolated Gold Nanoparticles. ACS Nano, 2015, 9, 4036-4042.	14.6	40
137	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
138	Carbonate Formation and Decomposition on Atomic Oxygen Precovered Au(111). Journal of the American Chemical Society, 2008, 130, 11250-11251.	13.7	39
139	Local density of states analysis using Bader decomposition for N2 and CO2 adsorbed on Pt(110)-(1â€‰Ã—â€‰2) electrodes. Journal of Chemical Physics, 2012, 137, 164705.	3.0	39
140	In Situ Raman Study of Phase Stability of Î±-Li₃V₂(PO₄)₃ upon Thermal and Laser Heating. Journal of Physical Chemistry C, 2013, 117, 11994-12002.	3.1	39
141	Computational Design of Alloy-Core@Shell Metal Nanoparticle Catalysts. ACS Catalysis, 2015, 5, 655-660.	11.2	39
142	Efficient CO Oxidation Using Dendrimer-Encapsulated Pt Nanoparticles Activated with <2% Cu Surface Atoms. ACS Nano, 2016, 10, 8760-8769.	14.6	39
143	Atomistic Simulations of Activated Processes in Materials. Annual Review of Materials Research, 2017, 47, 199-216.	9.3	38
144	Kinetic Monte Carlo simulations of Pd deposition and island growth on MgO(100). Surface Science, 2007, 601, 3133-3142.	1.9	37

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145	Ligand-Induced Structural Evolution of Pt₅₅ Nanoparticles: Amine versus Thiol. ACS Nano, 2011, 5, 8515-8522.	14.6	37
146	Molecular dynamics saddle search adaptive kinetic Monte Carlo. Journal of Chemical Physics, 2014, 140, 214110.	3.0	37
147	Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab Initio Molecular Dynamics and Nudged Elastic-Band Studies of NaBH₄ Hydrolysis. Journal of Physical Chemistry C, 2014, 118, 21385-21399.	3.1	37
148	Oxygen and Hydroxyl Species Induce Multiple Reaction Pathways for the Partial Oxidation of Allyl Alcohol on Gold. Journal of the American Chemical Society, 2014, 136, 6489-6498.	13.7	37
149	Why Silver Nanoparticles Are Effective for Olefin/Paraffin Separations. Journal of Physical Chemistry C, 2011, 115, 1811-1818.	3.1	35
150	Design of a Highly Nanodispersed Pdâ€“MgO/SiO₂ Composite Catalyst with Multifunctional Activity for CH₄ Reforming. ChemSusChem, 2012, 5, 1474-1481.	6.8	35
151	Correlating Structure and Function of Metal Nanoparticles for Catalysis. Surface Science, 2015, 640, 65-72.	1.9	35
152	Self-Assembled Cuâ€“Snâ€“S Nanotubes with High (De)Lithiation Performance. ACS Nano, 2017, 11, 10347-10356.	14.6	35
153	3d Transitionâ€Metalâ€Mediated Columbite Nanocatalysts for Decentralized Electrosynthesis of Hydrogen Peroxide. Small, 2021, 17, e2007249.	10.0	35
154	Structure Revealing H/D Exchange with Co-Adsorbed Hydrogen and Water on Gold. Journal of Physical Chemistry Letters, 2012, 3, 1894-1899.	4.6	34
155	Communication: From graphite to diamond: Reaction pathways of the phase transition. Journal of Chemical Physics, 2012, 137, 101101.	3.0	33
156	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
157	Intermetallic Pd₃Pb nanocubes with high selectivity for the 4-electron oxygen reduction reaction pathway. Nanoscale, 2020, 12, 2532-2541.	5.6	33
158	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
159	Pyrene: Hydrogenation, hydrogen evolution, and Ï€-band model. Journal of Chemical Physics, 2011, 134, 164703.	3.0	32
160	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
161	Cobalt Metalâ€“Cobalt Carbide Composite Microspheres for Water Reduction Electrocatalysis. ACS Applied Energy Materials, 2020, 3, 3909-3918.	5.1	32
162	Reviving reversible anion redox in 3d-transition-metal Li rich oxides by introducing surface defects. Nano Energy, 2020, 71, 104644.	16.0	31

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163	Electrochemical Properties of Three Li₂Ni₂TeO₆ Structural Polymorphs. Chemistry of Materials, 2019, 31, 9379-9388.	6.7	29
164	Synthesis and Dual-Mode Electrochromism of Anisotropic Monoclinic Nb₁₂O₂₉Colloidal Nanoplatelets. ACS Nano, 2020, 14, 10068-10082.	14.6	29
165	Gold boosts nitrate reduction and deactivation resistance to indium-promoted palladium catalysts. Applied Catalysis B: Environmental, 2022, 305, 121048.	20.2	29
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