Manos Mavrikakis

List of Publications by Year
in descending order

285	36,677	5558 82	3173 186
papers	citations	h-index	g-index

305	305	305	24182
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanistic Study of 1,2-Dichloroethane Hydrodechlorination on Cu-Rich Ptâ€“Cu Alloys: Combining Reaction Kinetics Experiments with DFT Calculations and Microkinetic Modeling. ACS Sustainable Chemistry and Engineering, 2022, 10, 1509-1523.	3.2	4
2	Solution-Phase Synthesis of PdH_{0.706} Nanocubes with Enhanced Stability and Activity toward Formic Acid Oxidation. Journal of the American Chemical Society, 2022, 144, 2556-2568.	6.6	42
3	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321.	23.0	195
4	Identifying hydroxylated copper dimers in SSZ-13 via UV-vis-NIR spectroscopy. Catalysis Science and Technology, 2022, 12, 2744-2748.	2.1	7
5	Trends in Formic Acid Electro-Oxidation on Transition Metals Alloyed with Platinum and Palladium. Journal of Physical Chemistry C, 2022, 126, 4374-4390.	1.5	8
6	A completely precious metalâ€“free alkaline fuel cell with enhanced performance using a carbon-coated nickel anode. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2119883119.	3.3	54
7	Phase-Controlled Synthesis of Ru Nanocrystals via Template-Directed Growth: Surface Energy versus Bulk Energy. Nano Letters, 2022, 22, 3591-3597.	4.5	7
8	Decomposition Kinetics of H₂O₂ on Pd Nanocrystals with Different Shapes and Surface Strains. ChemCatChem, 2022, 14, .	1.8	5
9	HCOOH Decomposition on Sub-Nanometer Pd6 Cluster Catalysts: The Effect of Defective Boron Nitride Supports Through First Principles. Applied Catalysis B: Environmental, 2021, 280, 119392.	10.8	19
10	Influence of multifluorophenyloxy terminus on the mesomorphism of the alkoxy and alkyl cyanobiphenyl compounds in search of new ambient nematic liquid crystals and mixtures. Liquid Crystals, 2021, 48, 672-688.	0.9	8
11	An automated cluster surface scanning method for exploring reaction paths on metal-cluster surfaces. Computational Materials Science, 2021, 186, 110010.	1.4	10
12	Physical Transformations of Noble-Metal Nanocrystals upon Thermal Activation. Accounts of Chemical Research, 2021, 54, 1-10.	7.6	23
13	Computational Methods in Heterogeneous Catalysis. Chemical Reviews, 2021, 121, 1007-1048.	23.0	198
14	Designing chemically selective liquid crystalline materials that respond to oxidizing gases. Journal of Materials Chemistry C, 2021, 9, 6507-6517.	2.7	9
15	Coupling the chemical reactivity of bimetallic surfaces to the orientations of liquid crystals. Materials Horizons, 2021, 8, 2050-2056.	6.4	8
16	Design of Chemoresponsive Soft Matter Using Hydrogen-Bonded Liquid Crystals. Materials, 2021, 14, 1055.	1.3	4
17	Effects of water on the kinetics of acetone hydrogenation over Pt and Ru catalysts. Journal of Catalysis, 2021, 403, 215-227.	3.1	10
18	Janus Nanocages of Platinumâ€Group Metals and Their Use as Effective Dualâ€Electrocatalysts. Angewandte Chemie, 2021, 133, 10472-10480.	1.6	4

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19	Janus Nanocages of Platinumâ€Group Metals and Their Use as Effective Dualâ€Electrocatalysts. Angewandte Chemie - International Edition, 2021, 60, 10384-10392.	7.2	33
20	Role of Hydrogen-bonded Bimolecular Formic Acidâ€“Formate Complexes for Formic Acid Decomposition on Copper: A Combined First-Principles and Microkinetic Modeling Study. ACS Catalysis, 2021, 11, 4349-4361.	5.5	19
21	Formic Acid Electrooxidation on Pt or Pd Monolayer on Transition-Metal Single Crystals: A First-Principles Structure Sensitivity Analysis. ACS Catalysis, 2021, 11, 5294-5309.	5.5	15
22	Structure sensitivity of ammonia electro-oxidation on transition metal surfaces: A first-principles study. Journal of Catalysis, 2021, 397, 137-147.	3.1	31
23	Atomistic insights into the nucleation and growth of platinum on palladium nanocrystals. Nature Communications, 2021, 12, 3215.	5.8	18
24	Hydrodechlorination of 1,2-Dichloroethane on Platinum Catalysts: Insights from Reaction Kinetics Experiments, Density Functional Theory, and Microkinetic Modeling. ACS Catalysis, 2021, 11, 7890-7905.	5.5	12
25	Thermodynamics Perspective on the Stepwise Conversion of Methane to Methanol over Cu-Exchanged SSZ-13. ACS Catalysis, 2021, 11, 7719-7734.	5.5	31
26	On the structure sensitivity of and CO coverage effects on formic acid decomposition on Pd surfaces. Surface Science, 2021, 709, 121846.	0.8	11
27	Mechanistic Similarities and Differences for Hydrogenation of Aromatic Heterocycles and Aliphatic Carbonyls on Sulfided Ru Nanoparticles. ACS Catalysis, 2021, 11, 12585-12608.	5.5	3
28	Steam-created grain boundaries for methane Câ€“H activation in palladium catalysts. Science, 2021, 373, 1518-1523.	6.0	105
29	Mechanism of methanol synthesis on Ni(110). Catalysis Science and Technology, 2021, 11, 3279-3294.	2.1	6
30	Introduction: Advanced Materials and Methods for Catalysis and Electrocatalysis by Transition Metals. Chemical Reviews, 2021, 121, 563-566.	23.0	33
31	Kinetically Controlled Synthesis of Pdâ€“Cu Janus Nanocrystals with Enriched Surface Structures and Enhanced Catalytic Activities toward CO₂ Reduction. Journal of the American Chemical Society, 2021, 143, 149-162.	6.6	77
32	Facile Synthesis of Palladiumâ€Based Nanocrystals with Different Crystal Phases and a Comparison of Their Catalytic Properties. Advanced Materials, 2021, 33, e2103801.	11.1	18
33	Synthesis and properties of fluorine tail-terminated cyanobiphenyls and terphenyls for chemoresponsive liquid crystals. Liquid Crystals, 2020, 47, 3-16.	0.9	17
34	New room temperature nematogens by cyano tail termination of alkoxy and alkylcyanobiphenyls and their anchoring behavior on metal salt-decorated surface. Liquid Crystals, 2020, 47, 540-556.	0.9	10
35	How coverage influences thermodynamic and kinetic isotope effects for H₂/D₂ dissociative adsorption on transition metals. Catalysis Science and Technology, 2020, 10, 671-689.	2.1	26
36	Molecular simulations of analyte partitioning and diffusion in liquid crystal sensors. Molecular Systems Design and Engineering, 2020, 5, 304-316.	1.7	14

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37	Facet-controlled Ptâ€“Ir nanocrystals with substantially enhanced activity and durability towards oxygen reduction. Materials Today, 2020, 35, 69-77.	8.3	45
38	Eliminating dissolution of platinum-based electrocatalysts at the atomic scale. Nature Materials, 2020, 19, 1207-1214.	13.3	127
39	Areas of opportunity related to design of chemical and biological sensors based on liquid crystals. Liquid Crystals Today, 2020, 29, 24-35.	2.3	30
40	Exploring driving forces for length growth in graphene nanoribbons during chemical vapor deposition of hydrocarbons on Ge(0Â0Â1) via kinetic Monte Carlo simulations. Applied Surface Science, 2020, 527, 146784.	3.1	8
41	Effect of strain on the reactivity of graphene films. Journal of Catalysis, 2020, 390, 67-71.	3.1	12
42	Combining Computational Modeling with Reaction Kinetics Experiments for Elucidating the In Situ Nature of the Active Site in Catalysis. Accounts of Chemical Research, 2020, 53, 1893-1904.	7.6	53
43	Formic Acid: A Hydrogen-Bonding Cocatalyst for Formate Decomposition. ACS Catalysis, 2020, 10, 10812-10825.	5.5	36
44	Site-dependent reactivity of MoS2 nanoparticles in hydrodesulfurization of thiophene. Nature Communications, 2020, 11, 4369.	5.8	44
45	ACS Catalysis Highlights Its Most Cited Papers From Around the Globe: United States. ACS Catalysis, 2020, 10, 15140-15141.	5.5	0
46	Comparing the performance of density functionals in describing the adsorption of atoms and small molecules on Ni(111). Surface Science, 2020, 700, 121675.	0.8	8
47	Binding of Organophosphorus Nerve Agents and Their Simulants to Metal Salts. ACS Applied Materials & Interfaces, 2020, 12, 30941-30953.	4.0	8
48	Pd3Ag(111) as a Model System for Hydrogen Separation Membranes: Combined Effects of CO Adsorption and Surface Termination on the Activation of Molecular Hydrogen. Topics in Catalysis, 2020, 63, 750-761.	1.3	13
49	Reaction Mechanism of Vapor-Phase Formic Acid Decomposition over Platinum Catalysts: DFT, Reaction Kinetics Experiments, and Microkinetic Modeling. ACS Catalysis, 2020, 10, 4112-4126.	5.5	51
50	How Noninnocent Spectator Species Improve the Oxygen Reduction Activity of Single-Atom Catalysts: Microkinetic Models from First-Principles Calculations. ACS Catalysis, 2020, 10, 9129-9135.	5.5	42
51	Bismuthene for highly efficient carbon dioxide electroreduction reaction. Nature Communications, 2020, 11, 1088.	5.8	278
52	Chloroform Hydrodechlorination on Palladium Surfaces: A Comparative DFT Study on Pd(111), Pd(100), and Pd(211). Topics in Catalysis, 2020, 63, 762-776.	1.3	17
53	A self-adjusting platinum surface for acetone hydrogenation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 3446-3450.	3.3	17
54	Computational Chemistry-Based Evaluation of Metal Salts and Metal Oxides for Application in Mercury-Capture Technologies. Industrial & Engineering Chemistry Research, 2020, 59, 9015-9022.	1.8	4

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55	Platinum and Palladium Monolayer Electrocatalysts for Formic Acid Oxidation. Topics in Catalysis, 2020, 63, 742-749.	1.3	17
56	Synthesis and properties of hydroxy tail-terminated cyanobiphenyl liquid crystals. Liquid Crystals, 2019, 46, 397-407.	0.9	22
57	Atomic and molecular adsorption on Ni(111). Surface Science, 2019, 679, 240-253.	0.8	41
58	Computational description of key spectroscopic features of zeolite SSZ-13. Physical Chemistry Chemical Physics, 2019, 21, 19065-19075.	1.3	11
59	Anisotropic Synthesis of Armchair Graphene Nanoribbon Arrays from Sub-5 nm Seeds at Variable Pitches on Germanium. Journal of Physical Chemistry Letters, 2019, 10, 4266-4272.	2.1	17
60	Correlation Between Reactivity and Oxidation State of Cobalt Oxide Catalysts for CO Preferential Oxidation. ACS Catalysis, 2019, 9, 8325-8336.	5.5	58
61	Effects of composition and morphology on the hydrogen storage properties of transition metal hydrides: Insights from PtPd nanoclusters. Nano Energy, 2019, 63, 103858.	8.2	15
62	Transition Metal Atoms Embedded in Graphene: How Nitrogen Doping Increases CO Oxidation Activity. ACS Catalysis, 2019, 9, 6864-6868.	5.5	72
63	BrÃ¸nstedâ€“Evansâ€“Polanyi relation for CO oxidation on metal oxides following the Marsâ€“van Krevelen mechanism. Journal of Catalysis, 2019, 377, 577-581.	3.1	33
64	UVâ€“Vis and Photoluminescence Spectroscopy to Understand the Coordination of Cu Cations in the Zeolite SSZ-13. Chemistry of Materials, 2019, 31, 9582-9592.	3.2	19
65	Identification of stable adsorption sites and diffusion paths on nanocluster surfaces: an automated scanning algorithm. Npj Computational Materials, 2019, 5, .	3.5	6
66	Kinetic Isolation between Turnovers on Au₁₈ Nanoclusters: Formic Acid Decomposition One Molecule at a Time. ACS Catalysis, 2019, 9, 9446-9457.	5.5	20
67	Amplification of Elementary Surface Reaction Steps on Transition Metal Surfaces Using Liquid Crystals: Dissociative Adsorption and Dehydrogenation. Journal of the American Chemical Society, 2019, 141, 16003-16013.	6.6	18
68	Mechanistic Role of the Protonâ€“Hydride Pair in Heteroarene Catalytic Hydrogenation. ACS Catalysis, 2019, 9, 9418-9437.	5.5	16
69	Hydrodechlorination of 1,2-dichloroethane on supported AgPd catalysts. Journal of Catalysis, 2019, 370, 241-250.	3.1	27
70	Anionic Single-Atom Catalysts for CO Oxidation: Support-Independent Activity at Low Temperatures. ACS Catalysis, 2019, 9, 1595-1604.	5.5	54
71	Facile One-Pot Synthesis of Pd@Pt_{1L} Octahedra with Enhanced Activity and Durability toward Oxygen Reduction. Chemistry of Materials, 2019, 31, 1370-1380.	3.2	41
72	On the nature of active sites for formic acid decomposition on gold catalysts. Catalysis Science and Technology, 2019, 9, 2836-2848.	2.1	24

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73	In situ, operando studies on the size and structure of supported Pt catalysts under supercritical conditions by simultaneous synchrotron-based X-ray techniques. Physical Chemistry Chemical Physics, 2019, 21, 11740-11747.	1.3	7
74	Iridiumâ€Based Cubic Nanocages with 1.1â€nmâ€Thick Walls: A Highly Efficient and Durable Electrocatalyst for Water Oxidation in an Acidic Medium. Angewandte Chemie - International Edition, 2019, 58, 7244-7248.	7.2	89
75	Iridiumâ€Based Cubic Nanocages with 1.1â€nmâ€Thick Walls: A Highly Efficient and Durable Electrocatalyst for Water Oxidation in an Acidic Medium. Angewandte Chemie, 2019, 131, 7322-7326.	1.6	12
76	Alignment of semiconducting graphene nanoribbons on vicinal Ge(001). Nanoscale, 2019, 11, 4864-4875.	2.8	26
77	Tightly Pitched sub-10 nm Graphene Nanoribbon Arrays via Seed Mediated Growth on Ge (001). ECS Transactions, 2019, 93, 121-124.	0.3	3
78	Single-atom gold oxo-clusters prepared in alkaline solutions catalyse the heterogeneous methanol self-coupling reactions. Nature Chemistry, 2019, 11, 1098-1105.	6.6	82
79	On the active site for electrocatalytic water splitting on late transition metals embedded in graphene. Catalysis Science and Technology, 2019, 9, 6793-6799.	2.1	9
80	Synthesis Gas Conversion over Rh/Mo Catalysts Prepared by Atomic Layer Deposition. ACS Catalysis, 2019, 9, 1810-1819.	5.5	33
81	Atomic and Molecular Adsorption on Ag(111). Journal of Physical Chemistry C, 2019, 123, 7551-7566.	1.5	39
82	(Invited) Electrocatalysis from First-Principles: Reaction Mechanisms and Ideas for Improved Materials. ECS Meeting Abstracts, 2019, , .	0.0	0
83	Direct Time-domain Observation of Attosecond Electron Dynamics in Solids using Attosecond Pulse Sequences. , 2019, , .		0
84	The role of iron-oxide aerosols and sunlight in the atmospheric reduction of Hg(II) species: A DFT+U study. Applied Catalysis B: Environmental, 2018, 234, 347-356.	10.8	10
85	Ethylene versus ethane: A DFT-based selectivity descriptor for efficient catalyst screening. Journal of Catalysis, 2018, 362, 18-24.	3.1	52
86	Ethylene Dimerization and Oligomerization to 1-Butene and Higher Olefins with Chromium-Promoted Cobalt on Carbon Catalyst. ACS Catalysis, 2018, 8, 2488-2497.	5.5	37
87	A DFT study of chlorine coverage over late transition metals and its implication on 1,2-dichloroethane hydrodechlorination. Catalysis Science and Technology, 2018, 8, 1555-1563.	2.1	16
88	Computational Chemistryâ€Guided Design of Selective Chemoresponsive Liquid Crystals Using Pyridine and Pyrimidine Functional Groups. Advanced Functional Materials, 2018, 28, 1703581.	7.8	27
89	Quantum chemical calculations to determine partitioning coefficients for HgCl2 on iron-oxide aerosols. Science of the Total Environment, 2018, 636, 580-587.	3.9	9
90	Ethane dehydrogenation on pristine and AlO_x decorated Pt stepped surfaces. Catalysis Science and Technology, 2018, 8, 2159-2174.	2.1	18

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91	Mechanistic Study of Nitric Oxide Reduction by Hydrogen on Pt(100) (I): A DFT Analysis of the Reaction Network. Journal of Physical Chemistry B, 2018, 122, 432-443.	1.2	29
92	Atomic and molecular adsorption on Fe(110). Surface Science, 2018, 667, 54-65.	0.8	49
93	The role of anions in adsorbate-induced anchoring transitions of liquid crystals on surfaces with discrete cation binding sites. Soft Matter, 2018, 14, 797-805.	1.2	27
94	Ir-Ni Bimetallic OER Catalysts Prepared by Controlled Ni Electrodeposition on Irpoly and Ir(111). Surfaces, 2018, 1, 165-186.	1.0	17
95	Structure Sensitivity of Formic Acid Electrooxidation on Transition Metal Surfaces: A First-Principles Study. Journal of the Electrochemical Society, 2018, 165, J3109-J3121.	1.3	39
96	Synthesis Gas Conversion over Rh-Mn-W_xC/SiO₂ Catalysts Prepared by Atomic Layer Deposition. ACS Catalysis, 2018, 8, 10707-10720.	5.5	17
97	Liquid Crystals with Interfacial Ordering that Enhances Responsiveness to Chemical Targets. Advanced Materials, 2018, 30, e1706707.	11.1	43
98	Synthesis of Ru Icosahedral Nanocages with a Face-Centered-Cubic Structure and Evaluation of Their Catalytic Properties. ACS Catalysis, 2018, 8, 6948-6960.	5.5	66
99	Atomic and Molecular Adsorption on Cu(111). Topics in Catalysis, 2018, 61, 736-750.	1.3	45
100	Redoxâ€Triggered Orientational Responses of Liquid Crystals to Chlorine Gas. Angewandte Chemie - International Edition, 2018, 57, 9665-9669.	7.2	39
101	Redoxâ€Triggered Orientational Responses of Liquid Crystals to Chlorine Gas. Angewandte Chemie, 2018, 130, 9813-9817.	1.6	11
102	Density functional theory study of thermodynamic and kinetic isotope effects of H2/D2 dissociative adsorption on transition metals. Catalysis Science and Technology, 2018, 8, 3321-3335.	2.1	26
103	(Keynote) Theoretical Inspirations from Radoslav Adzicâ€™s Electrocatalysis Work. ECS Meeting Abstracts, 2018, , .	0.0	0
104	Methane Conversion to Ethylene and Aromatics on PtSn Catalysts. ACS Catalysis, 2017, 7, 2088-2100.	5.5	93
105	Design of Chemoresponsive Liquid Crystals through Integration of Computational Chemistry and Experimental Studies. Chemistry of Materials, 2017, 29, 3563-3571.	3.2	33
106	Far above bandgap photonics: attosecond dynamics of highly excited electrons in materials. Proceedings of SPIE, 2017, , .	0.8	0
107	Understanding the Thermal Stability of Palladiumâ€“Platinum Coreâ€“Shell Nanocrystals by In Situ Transmission Electron Microscopy and Density Functional Theory. ACS Nano, 2017, 11, 4571-4581.	7.3	53
108	Thermal Stability of Metal Nanocrystals: An Investigation of the Surface and Bulk Reconstructions of Pd Concave Icosahedra. Nano Letters, 2017, 17, 3655-3661.	4.5	43

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109	Boron Nitrideâ€supported Subâ€nanometer Pd 6 Clusters for Formic Acid Decomposition: A DFT Study. ChemCatChem, 2017, 9, 1610-1620.	1.8	23
110	Synthesis Gas Conversion over Rh-Based Catalysts Promoted by Fe and Mn. ACS Catalysis, 2017, 7, 4550-4563.	5.5	51
111	On the Preferred Active Sites of Promoted MoS₂ for Hydrodesulfurization with Minimal Organonitrogen Inhibition. ACS Catalysis, 2017, 7, 501-509.	5.5	78
112	Facile Synthesis of Ru-Based Octahedral Nanocages with Ultrathin Walls in a Face-Centered Cubic Structure. Chemistry of Materials, 2017, 29, 9227-9237.	3.2	55
113	Toward rational nanoparticle synthesis: predicting surface intermixing in bimetallic alloy nanocatalysts. Nanoscale, 2017, 9, 15005-15017.	2.8	24
114	Sequential-Optimization-Based Framework for Robust Modeling and Design of Heterogeneous Catalytic Systems. Journal of Physical Chemistry C, 2017, 121, 25847-25863.	1.5	42
115	Distinguishing attosecond electronâ€“electron scattering and screening in transition metals. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E5300-E5307.	3.3	55
116	Optimization Methods for Catalyst Design. Computer Aided Chemical Engineering, 2016, 38, 295-300.	0.3	3
117	Chloroform Hydrodechlorination over Palladiumâ€“Gold Catalysts: A Firstâ€Principles DFT Study. ChemCatChem, 2016, 8, 1739-1746.	1.8	12
118	The nature of the Fe-graphene interface at the nanometer level. AIP Conference Proceedings, 2016, , .	0.3	0
119	DFT Insights into the Competitive Adsorption of Sulfur- and Nitrogen-Containing Compounds and Hydrocarbons on Co-Promoted Molybdenum Sulfide Catalysts. ACS Catalysis, 2016, 6, 2904-2917.	5.5	66
120	Synthesis and Characterization of Ptâ€“Ag Alloy Nanocages with Enhanced Activity and Durability toward Oxygen Reduction. Nano Letters, 2016, 16, 6644-6649.	4.5	150
121	Synthesis and Characterization of Ru Cubic Nanocages with a Face-Centered Cubic Structure by Templating with Pd Nanocubes. Nano Letters, 2016, 16, 5310-5317.	4.5	110
122	Ab initio molecular dynamics of solvation effects on reactivity at electrified interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4937-45.	3.3	57
123	On the Structure Sensitivity of Formic Acid Decomposition on Cu Catalysts. Topics in Catalysis, 2016, 59, 1580-1588.	1.3	37
124	Towards first-principles molecular design of liquid crystal-based chemoresponsive systems. Nature Communications, 2016, 7, 13338.	5.8	34
125	Adsorption of Small Alkanes on ZSM-5 Zeolites: Influence of BrÃ¸nsted Sites. Journal of Physical Chemistry C, 2016, 120, 12132-12138.	1.5	25
126	Direct time-domain observation of attosecond final-state lifetimes in photoemission from solids. Science, 2016, 353, 62-67.	6.0	181

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127	Identification of O-rich structures on platinum(111)-supported ultrathin iron oxide films. Surface Science, 2016, 652, 261-268.	0.8	27
128	Heterogeneous Reduction Pathways for Hg(II) Species on Dry Aerosols: A First-Principles Computational Study. Journal of Physical Chemistry A, 2016, 120, 2106-2113.	1.1	10
129	Active sites and mechanisms for H ₂ O ₂ decomposition over Pd catalysts. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E1973-82.	3.3	171
130	Dimethyl ether electro-oxidation on platinum surfaces. Nano Energy, 2016, 29, 428-438.	8.2	17
131	Density functional theory studies of HCOOH decomposition on Pd(111). Surface Science, 2016, 650, 111-120.	0.8	70
132	HCOOH decomposition on Pt(111): A DFT study. Surface Science, 2016, 648, 201-211.	0.8	54
133	Controlling the electronic structure of graphene using surface-adsorbate interactions. Physical Review B, 2015, 92, .	1.1	8
134	Adsorption of nitrogenâ€•and sulfurâ€containing compounds on NiMoS for hydrotreating reactions: A DFT and vdWâ€corrected study. AICHE Journal, 2015, 61, 4036-4050.	1.8	39
135	A Comprehensive Study of Formic Acid Oxidation on Palladium Nanocrystals with Different Types of Facets and Twin Defects. ChemCatChem, 2015, 7, 2077-2084.	1.8	111
136	Direct Visualization of Catalytically Active Sites at the FeOâ€“Pt(111) Interface. ACS Nano, 2015, 9, 7804-7814.	7.3	67
137	Computational chemistry for NH3 synthesis, hydrotreating, and NO reduction: Three topics of special interest to Haldor TopsÃ¸e. Journal of Catalysis, 2015, 328, 26-35.	3.1	15
138	An Adsorption Study of CH₄ on ZSM-5, MOR, and ZSM-12 Zeolites. Journal of Physical Chemistry C, 2015, 119, 28970-28978.	1.5	32
139	On the Structure Sensitivity of Dimethyl Ether Electro-oxidation on Eight FCC Metals: A First-Principles Study. Topics in Catalysis, 2015, 58, 1159-1173.	1.3	13
140	Atomic Layer-by-Layer Deposition of Platinum on Palladium Octahedra for Enhanced Catalysts toward the Oxygen Reduction Reaction. ACS Nano, 2015, 9, 2635-2647.	7.3	209
141	Stability of surface and subsurface hydrogen on and in Au/Ni near-surface alloys. Surface Science, 2015, 640, 190-197.	0.8	4
142	Platinum-based nanocages with subnanometer-thick walls and well-defined, controllable facets. Science, 2015, 349, 412-416.	6.0	854
143	Palladiumâ€“platinum core-shell icosahedra with substantially enhanced activity and durability towards oxygen reduction. Nature Communications, 2015, 6, 7594.	5.8	440
144	Electrocatalytic Oxidation of Ammonia on Transition-Metal Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 14692-14701.	1.5	137

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145	Direct Synthesis of Hydrogen Peroxide Over Auâ€“Pd Catalysts Prepared by Electroless Deposition. Catalysis Letters, 2015, 145, 2057-2065.	1.4	11
146	The nature of the Feâ€“graphene interface at the nanometer level. Nanoscale, 2015, 7, 2450-2460.	2.8	44
147	Adsorbate Diffusion on Transition Metal Nanoparticles. Nano Letters, 2015, 15, 629-634.	4.5	26
148	A tribute to R. Byron Bird. AICHE Journal, 2014, 60, 1218-1218.	1.8	0
149	Catalytically active Au-O(OH) _x - species stabilized by alkali ions on zeolites and mesoporous oxides. Science, 2014, 346, 1498-1501.	6.0	544
150	Advanced solution methods for microkinetic models of catalytic reactions: A methanol synthesis case study. AICHE Journal, 2014, 60, 1336-1346.	1.8	19
151	Formic acid decomposition on Au catalysts: DFT, microkinetic modeling, and reaction kinetics experiments. AICHE Journal, 2014, 60, 1303-1319.	1.8	87
152	Highly Crystalline Multimetallic Nanoframes with Three-Dimensional Electrocatalytic Surfaces. Science, 2014, 343, 1339-1343.	6.0	2,376
153	Atomic Layer-by-Layer Deposition of Pt on Pd Nanocubes for Catalysts with Enhanced Activity and Durability toward Oxygen Reduction. Nano Letters, 2014, 14, 3570-3576.	4.5	448
154	Atomic and Molecular Adsorption on Re(0001). Topics in Catalysis, 2014, 57, 54-68.	1.3	28
155	Trends in Formic Acid Decomposition on Model Transition Metal Surfaces: A Density Functional Theory study. ACS Catalysis, 2014, 4, 4434-4445.	5.5	190
156	First-Principles Mechanistic Analysis of Dimethyl Ether Electro-Oxidation on Monometallic Single-Crystal Surfaces. Journal of Physical Chemistry C, 2014, 118, 24199-24211.	1.5	23
157	Water clustering on nanostructured iron oxide films. Nature Communications, 2014, 5, 4193.	5.8	65
158	Density Functional Theory Calculations and Analysis of Reaction Pathways for Reduction of Nitric Oxide by Hydrogen on Pt(111). ACS Catalysis, 2014, 4, 3307-3319.	5.5	93
159	Atomic and molecular adsorption on Au(111). Surface Science, 2014, 627, 57-69.	0.8	78
160	On the composition of bimetallic near-surface alloys in the presence of oxygen and carbon monoxide. Catalysis Communications, 2014, 52, 65-71.	1.6	26
161	Significant Quantum Effects in Hydrogen Activation. ACS Nano, 2014, 8, 4827-4835.	7.3	44
162	Facile Synthesis of Palladium Right Bipyramids and Their Use as Seeds for Overgrowth and as Catalysts for Formic Acid Oxidation. Journal of the American Chemical Society, 2013, 135, 15706-15709.	6.6	139

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163	Tuning the Catalytic Activity of Ru@Pt Coreâ€“Shell Nanoparticles for the Oxygen Reduction Reaction by Varying the Shell Thickness. Journal of Physical Chemistry C, 2013, 117, 1748-1753.	1.5	140
164	Mechanistic Studies of Oxygen Reduction by Hydrogen on PdAg(110). ACS Catalysis, 2013, 3, 1622-1632.	5.5	32
165	Atomic and molecular adsorption on Ru(0001). Surface Science, 2013, 614, 64-74.	0.8	71
166	Stabilization of Copper Catalysts for Liquidâ€Phase Reactions by Atomic Layer Deposition. Angewandte Chemie - International Edition, 2013, 52, 13808-13812.	7.2	162
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