Manos Mavrikakis

List of Publications by Year in Descending Order

281 papers	30,512 citations	76 h-index	171 g-index
305 ext. papers	33,559 ext. citations	9.4 avg, IF	7.42 L-index

#	Paper	IF	Citations
281	Mechanistic Study of 1,2-Dichloroethane Hydrodechlorination on Cu-Rich PtCu Alloys: Combining Reaction Kinetics Experiments with DFT Calculations and Microkinetic Modeling. *ACS Sustainable Chemistry and Engineering*, **2022**, 10, 1509-1523	8.3	1
280	Solution-Phase Synthesis of PdH Nanocubes with Enhanced Stability and Activity toward Formic Acid Oxidation.. *Journal of the American Chemical Society*, **2022**,	16.4	8
279	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies.. *Chemical Reviews*, **2022**,	68.1	25
278	Trends in Formic Acid Electro-Oxidation on Transition Metals Alloyed with Platinum and Palladium. *Journal of Physical Chemistry C*, **2022**, 126, 4374-4390	3.8	0
277	A completely precious metal-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	11.5	2
276	Facile Synthesis of Palladium-Based Nanocrystals with Different Crystal Phases and a Comparison of Their Catalytic Properties. *Advanced Materials*, **2021**, 33, e2103801	24	4
275	Kinetically Controlled Synthesis of Pd-Cu Janus Nanocrystals with Enriched Surface Structures and Enhanced Catalytic Activities toward CO Reduction. *Journal of the American Chemical Society*, **2021**, 143, 149-162	16.4	24
274	Effects of water on the kinetics of acetone hydrogenation over Pt and Ru catalysts. *Journal of Catalysis*, **2021**, 403, 215-215	7.3	1
273	Janus Nanocages of Platinum-Group Metals and Their Use as Effective Dual-Electrocatalysts. *Angewandte Chemie*, **2021**, 133, 10472-10480	3.6	2
272	Janus Nanocages of Platinum-Group Metals and Their Use as Effective Dual-Electrocatalysts. *Angewandte Chemie - International Edition*, **2021**, 60, 10384-10392	16.4	12
271	Role of Hydrogen-bonded Bimolecular Formic Acid–Formate Complexes for Formic Acid Decomposition on Copper: A Combined First-Principles and Microkinetic Modeling Study. *ACS Catalysis*, **2021**, 11, 4349-4361	13.1	8
270	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	13.1	5
269	Structure sensitivity of ammonia electro-oxidation on transition metal surfaces: A first-principles study. *Journal of Catalysis*, **2021**, 397, 137-147	7.3	4
268	Atomistic insights into the nucleation and growth of platinum on palladium nanocrystals. *Nature Communications*, **2021**, 12, 3215	17.4	4
267	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	13.1	6
266	Thermodynamics Perspective on the Stepwise Conversion of Methane to Methanol over Cu-Exchanged SSZ-13. *ACS Catalysis*, **2021**, 11, 7719-7734	13.1	9
265	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	21.8	9

264	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	2.3	1
263	An automated cluster surface scanning method for exploring reaction paths on metal-cluster surfaces. *Computational Materials Science*, **2021**, 186, 110010	3.2	2
262	Physical Transformations of Noble-Metal Nanocrystals upon Thermal Activation. *Accounts of Chemical Research*, **2021**, 54, 1-10	24.3	8
261	Computational Methods in Heterogeneous Catalysis. *Chemical Reviews*, **2021**, 121, 1007-1048	68.1	61
260	Designing chemically selective liquid crystalline materials that respond to oxidizing gases. *Journal of Materials Chemistry C*, **2021**, 9, 6507-6517	7.1	2
259	Coupling the chemical reactivity of bimetallic surfaces to the orientations of liquid crystals. *Materials Horizons*, **2021**, 8, 2050-2056	14.4	1
258	Design of Chemoresponsive Soft Matter Using Hydrogen-Bonded Liquid Crystals. *Materials*, **2021**, 14,	3.5	2
257	On the structure sensitivity of and CO coverage effects on formic acid decomposition on Pd surfaces. *Surface Science*, **2021**, 709, 121846	1.8	6
256	Steam-created grain boundaries for methane C-H activation in palladium catalysts. *Science*, **2021**, 373, 1518-1523	33.3	15
255	Mechanism of methanol synthesis on Ni(110). *Catalysis Science and Technology*, **2021**, 11, 3279-3294	5.5	2
254	Comparing the performance of density functionals in describing the adsorption of atoms and small molecules on Ni(111). *Surface Science*, **2020**, 700, 121675	1.8	3
253	Binding of Organophosphorus Nerve Agents and Their Simulants to Metal Salts. *ACS Applied Materials & Interfaces*, **2020**, 12, 30941-30953	9.5	3
252	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	2.3	6
251	Reaction Mechanism of Vapor-Phase Formic Acid Decomposition over Platinum Catalysts: DFT, Reaction Kinetics Experiments, and Microkinetic Modeling. *ACS Catalysis*, **2020**, 10, 4112-4126	13.1	36
250	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	13.1	26
249	Bismuthene for highly efficient carbon dioxide electroreduction reaction. *Nature Communications*, **2020**, 11, 1088	17.4	125
248	Chloroform Hydrodechlorination on Palladium Surfaces: A Comparative DFT Study on Pd(111), Pd(100), and Pd(211). *Topics in Catalysis*, **2020**, 63, 762-776	2.3	7
247	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	11.5	13

246	Computational Chemistry-Based Evaluation of Metal Salts and Metal Oxides for Application in Mercury-Capture Technologies. *Industrial & Engineering Chemistry Research*, **2020**, 59, 9015-9022	3.9	4
245	Platinum and Palladium Monolayer Electrocatalysts for Formic Acid Oxidation. *Topics in Catalysis*, **2020**, 63, 742-749	2.3	9
244	How coverage influences thermodynamic and kinetic isotope effects for H2/D2 dissociative adsorption on transition metals. *Catalysis Science and Technology*, **2020**, 10, 671-689	5.5	14
243	Molecular simulations of analyte partitioning and diffusion in liquid crystal sensors. *Molecular Systems Design and Engineering*, **2020**, 5, 304-316	4.6	6
242	Facet-controlled Pt□ nanocrystals with substantially enhanced activity and durability towards oxygen reduction. *Materials Today*, **2020**, 35, 69-77	21.8	20
241	Eliminating dissolution of platinum-based electrocatalysts at the atomic scale. *Nature Materials*, **2020**, 19, 1207-1214	27	57
240	Areas of opportunity related to design of chemical and biological sensors based on liquid crystals. *Liquid Crystals Today*, **2020**, 29, 24-35	1.9	13
239	Exploring driving forces for length growth in graphene nanoribbons during chemical vapor deposition of hydrocarbons on Ge(0 0 1) via kinetic Monte Carlo simulations. *Applied Surface Science*, **2020**, 527, 146784	6.7	4
238	Effect of strain on the reactivity of graphene films. *Journal of Catalysis*, **2020**, 390, 67-71	7.3	7
237	Combining Computational Modeling with Reaction Kinetics Experiments for Elucidating the Nature of the Active Site in Catalysis. *Accounts of Chemical Research*, **2020**, 53, 1893-1904	24.3	27
236	Formic Acid: A Hydrogen-Bonding Cocatalyst for Formate Decomposition. *ACS Catalysis*, **2020**, 10, 10812-10825	13.1	19
235	Site-dependent reactivity of MoS nanoparticles in hydrodesulfurization of thiophene. *Nature Communications*, **2020**, 11, 4369	17.4	17
234	ACS Catalysis Highlights Its Most Cited Papers From Around the Globe: United States. *ACS Catalysis*, **2020**, 10, 15140-15141	13.1	
233	Synthesis and properties of fluorine tail-terminated cyanobiphenyls and terphenyls for chemoresponsive liquid crystals. *Liquid Crystals*, **2020**, 47, 3-16	2.3	6
232	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	2.3	3
231	Identification of stable adsorption sites and diffusion paths on nanocluster surfaces: an automated scanning algorithm. *Npj Computational Materials*, **2019**, 5,	10.9	4
230	Kinetic Isolation between Turnovers on Au18 Nanoclusters: Formic Acid Decomposition One Molecule at a Time. *ACS Catalysis*, **2019**, 9, 9446-9457	13.1	10
229	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	16.4	9

228	Mechanistic Role of the Proton–Hydride Pair in Heteroarene Catalytic Hydrogenation. *ACS Catalysis*, **2019**, 9, 9418-9437	13.1	10
227	Hydrodechlorination of 1,2-dichloroethane on supported AgPd catalysts. *Journal of Catalysis*, **2019**, 370, 241-250	7.3	16
226	Anionic Single-Atom Catalysts for CO Oxidation: Support-Independent Activity at Low Temperatures. *ACS Catalysis*, **2019**, 9, 1595-1604	13.1	39
225	Facile One-Pot Synthesis of Pd@Pt1L Octahedra with Enhanced Activity and Durability toward Oxygen Reduction. *Chemistry of Materials*, **2019**, 31, 1370-1380	9.6	29
224	On the nature of active sites for formic acid decomposition on gold catalysts. *Catalysis Science and Technology*, **2019**, 9, 2836-2848	5.5	13
223	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	3.6	5
222	Iridium-Based Cubic Nanocages with 1.1-nm-Thick Walls: A Highly Efficient and Durable Electrocatalyst for Water Oxidation in an Acidic Medium. *Angewandte Chemie - International Edition*, **2019**, 58, 7244-7248	16.4	59
221	Iridium-Based Cubic Nanocages with 1.1-nm-Thick Walls: A Highly Efficient and Durable Electrocatalyst for Water Oxidation in an Acidic Medium. *Angewandte Chemie*, **2019**, 131, 7322-7326	3.6	6
220	Alignment of semiconducting graphene nanoribbons on vicinal Ge(001). *Nanoscale*, **2019**, 11, 4864-4875	7.7	20
219	Synthesis and properties of hydroxy tail-terminated cyanobiphenyl liquid crystals. *Liquid Crystals*, **2019**, 46, 397-407	2.3	11
218	Atomic and molecular adsorption on Ni(111). *Surface Science*, **2019**, 679, 240-253	1.8	25
217	Computational description of key spectroscopic features of zeolite SSZ-13. *Physical Chemistry Chemical Physics*, **2019**, 21, 19065-19075	3.6	5
216	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	6.4	12
215	Correlation Between Reactivity and Oxidation State of Cobalt Oxide Catalysts for CO Preferential Oxidation. *ACS Catalysis*, **2019**, 9, 8325-8336	13.1	29
214	Effects of composition and morphology on the hydrogen storage properties of transition metal hydrides: Insights from PtPd nanoclusters. *Nano Energy*, **2019**, 63, 103858	17.1	9
213	Transition Metal Atoms Embedded in Graphene: How Nitrogen Doping Increases CO Oxidation Activity. *ACS Catalysis*, **2019**, 9, 6864-6868	13.1	44
212	Brønsted–Evans–Polanyi relation for CO oxidation on metal oxides following the Mars–van Krevelen mechanism. *Journal of Catalysis*, **2019**, 377, 577-581	7.3	22
211	UV–Vis and Photoluminescence Spectroscopy to Understand the Coordination of Cu Cations in the Zeolite SSZ-13. *Chemistry of Materials*, **2019**, 31, 9582-9592	9.6	10

210	Tightly Pitched sub-10 nm Graphene Nanoribbon Arrays via Seed Mediated Growth on Ge (001). *ECS Transactions*, **2019**, 93, 121-124	1	3
209	Single-atom gold oxo-clusters prepared in alkaline solutions catalyse the heterogeneous methanol self-coupling reactions. *Nature Chemistry*, **2019**, 11, 1098-1105	17.6	44
208	On the active site for electrocatalytic water splitting on late transition metals embedded in graphene. *Catalysis Science and Technology*, **2019**, 9, 6793-6799	5.5	8
207	Synthesis Gas Conversion over Rh/Mo Catalysts Prepared by Atomic Layer Deposition. *ACS Catalysis* , **2019**, 9, 1810-1819	13.1	22
206	Atomic and Molecular Adsorption on Ag(111). *Journal of Physical Chemistry C*, **2019**, 123, 7551-7566	3.8	26
205	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	21.8	7
204	Ethylene versus ethane: A DFT-based selectivity descriptor for efficient catalyst screening. *Journal of Catalysis*, **2018**, 362, 18-24	7.3	39
203	Ethylene Dimerization and Oligomerization to 1-Butene and Higher Olefins with Chromium-Promoted Cobalt on Carbon Catalyst. *ACS Catalysis*, **2018**, 8, 2488-2497	13.1	27
202	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	5.5	11
201	Computational Chemistry-Guided Design of Selective Chemoresponsive Liquid Crystals Using Pyridine and Pyrimidine Functional Groups. *Advanced Functional Materials*, **2018**, 28, 1703581	15.6	23
200	Quantum chemical calculations to determine partitioning coefficients for HgCl on iron-oxide aerosols. *Science of the Total Environment*, **2018**, 636, 580-587	10.2	8
199	Ethane dehydrogenation on pristine and AlOx decorated Pt stepped surfaces. *Catalysis Science and Technology*, **2018**, 8, 2159-2174	5.5	12
198	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	3.4	21
197	Atomic and molecular adsorption on Fe(110). *Surface Science*, **2018**, 667, 54-65	1.8	27
196	Redox-Triggered Orientational Responses of Liquid Crystals to Chlorine Gas. *Angewandte Chemie - International Edition*, **2018**, 57, 9665-9669	16.4	21
195	Redox-Triggered Orientational Responses of Liquid Crystals to Chlorine Gas. *Angewandte Chemie*, **2018**, 130, 9813-9817	3.6	6
194	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	5.5	19
193	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	3.6	20

192	Ir-Ni Bimetallic OER Catalysts Prepared by Controlled Ni Electrodeposition on Irpoly and Ir(111). *Surfaces*, **2018**, 1, 165-186	2.9	7
191	Structure Sensitivity of Formic Acid Electrooxidation on Transition Metal Surfaces: A First-Principles Study. *Journal of the Electrochemical Society*, **2018**, 165, J3109-J3121	3.9	24
190	Synthesis Gas Conversion over Rh-Mn-WxC/SiO2 Catalysts Prepared by Atomic Layer Deposition. *ACS Catalysis*, **2018**, 8, 10707-10720	13.1	15
189	Liquid Crystals with Interfacial Ordering that Enhances Responsiveness to Chemical Targets. *Advanced Materials*, **2018**, 30, e1706707	24	28
188	Synthesis of Ru Icosahedral Nanocages with a Face-Centered-Cubic Structure and Evaluation of Their Catalytic Properties. *ACS Catalysis*, **2018**, 8, 6948-6960	13.1	45
187	Atomic and Molecular Adsorption on Cu(111). *Topics in Catalysis*, **2018**, 61, 736-750	2.3	25
186	Methane Conversion to Ethylene and Aromatics on PtSn Catalysts. *ACS Catalysis*, **2017**, 7, 2088-2100	13.1	73
185	Design of Chemoresponsive Liquid Crystals through Integration of Computational Chemistry and Experimental Studies. *Chemistry of Materials*, **2017**, 29, 3563-3571	9.6	28
184	Understanding the Thermal Stability of Palladium-Platinum Core-Shell Nanocrystals by In Situ Transmission Electron Microscopy and Density Functional Theory. *ACS Nano*, **2017**, 11, 4571-4581	16.7	42
183	Thermal Stability of Metal Nanocrystals: An Investigation of the Surface and Bulk Reconstructions of Pd Concave Icosahedra. *Nano Letters*, **2017**, 17, 3655-3661	11.5	39
182	Boron Nitride-supported Sub-nanometer Pd6 Clusters for Formic Acid Decomposition: A DFT Study. *ChemCatChem*, **2017**, 9, 1610-1620	5.2	22
181	Synthesis Gas Conversion over Rh-Based Catalysts Promoted by Fe and Mn. *ACS Catalysis*, **2017**, 7, 4550-4563	13.1	42
180	On the Preferred Active Sites of Promoted MoS2 for Hydrodesulfurization with Minimal Organonitrogen Inhibition. *ACS Catalysis*, **2017**, 7, 501-509	13.1	53
179	Facile Synthesis of Ru-Based Octahedral Nanocages with Ultrathin Walls in a Face-Centered Cubic Structure. *Chemistry of Materials*, **2017**, 29, 9227-9237	9.6	45
178	Toward rational nanoparticle synthesis: predicting surface intermixing in bimetallic alloy nanocatalysts. *Nanoscale*, **2017**, 9, 15005-15017	7.7	20
177	Sequential-Optimization-Based Framework for Robust Modeling and Design of Heterogeneous Catalytic Systems. *Journal of Physical Chemistry C*, **2017**, 121, 25847-25863	3.8	30
176	Distinguishing attosecond electron-electron scattering and screening in transition metals. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E5300-E5307	11.5	47
175	Optimization Methods for Catalyst Design. *Computer Aided Chemical Engineering*, **2016**, 38, 295-300	0.6	2

174	On the Structure Sensitivity of Formic Acid Decomposition on Cu Catalysts. *Topics in Catalysis*, **2016**, 59, 1580-1588	2.3	25
173	Towards first-principles molecular design of liquid crystal-based chemoresponsive systems. *Nature Communications*, **2016**, 7, 13338	17.4	25
172	Adsorption of Small Alkanes on ZSM-5 Zeolites: Influence of Brønsted Sites. *Journal of Physical Chemistry C*, **2016**, 120, 12132-12138	3.8	18
171	Direct time-domain observation of attosecond final-state lifetimes in photoemission from solids. *Science*, **2016**, 353, 62-7	33.3	126
170	Identification of O-rich structures on platinum(111)-supported ultrathin iron oxide films. *Surface Science*, **2016**, 652, 261-268	1.8	22
169	Heterogeneous Reduction Pathways for Hg(II) Species on Dry Aerosols: A First-Principles Computational Study. *Journal of Physical Chemistry A*, **2016**, 120, 2106-13	2.8	8
168	Active sites and mechanisms for HCOOH decomposition over Pd catalysts. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E1973-82	11.5	122
167	Dimethyl ether electro-oxidation on platinum surfaces. *Nano Energy*, **2016**, 29, 428-438	17.1	14
166	Density functional theory studies of HCOOH decomposition on Pd(111). *Surface Science*, **2016**, 650, 111-120	1.8	55
165	HCOOH decomposition on Pt(111): A DFT study. *Surface Science*, **2016**, 648, 201-211	1.8	44
164	Chloroform Hydrodechlorination over Palladium–Gold Catalysts: A First-Principles DFT Study. *ChemCatChem*, **2016**, 8, 1739-1746	5.2	8
163	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	13.1	58
162	Synthesis and Characterization of Pt-Ag Alloy Nanocages with Enhanced Activity and Durability toward Oxygen Reduction. *Nano Letters*, **2016**, 16, 6644-6649	11.5	132
161	Synthesis and Characterization of Ru Cubic Nanocages with a Face-Centered Cubic Structure by Templating with Pd Nanocubes. *Nano Letters*, **2016**, 16, 5310-7	11.5	84
160	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	11.5	50
159	NANOCATALYSTS. Platinum-based nanocages with subnanometer-thick walls and well-defined, controllable facets. *Science*, **2015**, 349, 412-6	33.3	724
158	Palladium-platinum core-shell icosahedra with substantially enhanced activity and durability towards oxygen reduction. *Nature Communications*, **2015**, 6, 7594	17.4	365
157	Electrocatalytic Oxidation of Ammonia on Transition-Metal Surfaces: A First-Principles Study. *Journal of Physical Chemistry C*, **2015**, 119, 14692-14701	3.8	84

156	Direct Synthesis of Hydrogen Peroxide Over AuPd Catalysts Prepared by Electroless Deposition. *Catalysis Letters*, **2015**, 145, 2057-2065	2.8	10
155	The nature of the Fe-graphene interface at the nanometer level. *Nanoscale*, **2015**, 7, 2450-60	7.7	33
154	Adsorbate diffusion on transition metal nanoparticles. *Nano Letters*, **2015**, 15, 629-34	11.5	22
153	Controlling the electronic structure of graphene using surface-adsorbate interactions. *Physical Review B*, **2015**, 92,	3.3	6
152	Adsorption of nitrogen- and sulfur-containing compounds on NiMoS for hydrotreating reactions: A DFT and vdW-corrected study. *AICHE Journal*, **2015**, 61, 4036-4050	3.6	34
151	A Comprehensive Study of Formic Acid Oxidation on Palladium Nanocrystals with Different Types of Facets and Twin Defects. *ChemCatChem*, **2015**, 7, 2077-2084	5.2	91
150	Direct Visualization of Catalytically Active Sites at the FeO-Pt(111) Interface. *ACS Nano*, **2015**, 9, 7804-14	16.7	54
149	Computational chemistry for NH3 synthesis, hydrotreating, and NOx reduction: Three topics of special interest to Haldor Topsø. *Journal of Catalysis*, **2015**, 328, 26-35	7.3	9
148	An Adsorption Study of CH4 on ZSM-5, MOR, and ZSM-12 Zeolites. *Journal of Physical Chemistry C*, **2015**, 119, 28970-28978	3.8	25
147	On the Structure Sensitivity of Dimethyl Ether Electro-oxidation on Eight FCC Metals: A First-Principles Study. *Topics in Catalysis*, **2015**, 58, 1159-1173	2.3	11
146	Atomic layer-by-layer deposition of platinum on palladium octahedra for enhanced catalysts toward the oxygen reduction reaction. *ACS Nano*, **2015**, 9, 2635-47	16.7	180
145	Stability of surface and subsurface hydrogen on and in Au/Ni near-surface alloys. *Surface Science*, **2015**, 640, 190-197	1.8	3
144	Advanced solution methods for microkinetic models of catalytic reactions: A methanol synthesis case study. *AICHE Journal*, **2014**, 60, 1336-1346	3.6	16
143	Formic acid decomposition on Au catalysts: DFT, microkinetic modeling, and reaction kinetics experiments. *AICHE Journal*, **2014**, 60, 1303-1319	3.6	78
142	Highly crystalline multimetallic nanoframes with three-dimensional electrocatalytic surfaces. *Science*, **2014**, 343, 1339-43	33.3	1989
141	Atomic layer-by-layer deposition of Pt on Pd nanocubes for catalysts with enhanced activity and durability toward oxygen reduction. *Nano Letters*, **2014**, 14, 3570-6	11.5	380
140	Atomic and Molecular Adsorption on Re(0001). *Topics in Catalysis*, **2014**, 57, 54-68	2.3	22
139	Trends in Formic Acid Decomposition on Model Transition Metal Surfaces: A Density Functional Theory study. *ACS Catalysis*, **2014**, 4, 4434-4445	13.1	159

138	First-Principles Mechanistic Analysis of Dimethyl Ether Electro-Oxidation on Monometallic Single-Crystal Surfaces. *Journal of Physical Chemistry C*, **2014**, 118, 24199-24211	3.8	17
137	Water clustering on nanostructured iron oxide films. *Nature Communications*, **2014**, 5, 4193	17.4	53
136	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	13.1	59
135	Atomic and molecular adsorption on Au(111). *Surface Science*, **2014**, 627, 57-69	1.8	58
134	On the composition of bimetallic near-surface alloys in the presence of oxygen and carbon monoxide. *Catalysis Communications*, **2014**, 52, 65-71	3.2	21
133	Significant quantum effects in hydrogen activation. *ACS Nano*, **2014**, 8, 4827-35	16.7	35
132	Catalytically active Au-O(OH)x-species stabilized by alkali ions on zeolites and mesoporous oxides. *Science*, **2014**, 346, 1498-501	33.3	437
131	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, 15706-9	16.4	125
130	Tuning the Catalytic Activity of Core–Shell Nanoparticles for the Oxygen Reduction Reaction by Varying the Shell Thickness. *Journal of Physical Chemistry C*, **2013**, 117, 1748-1753	3.8	120
129	Mechanistic Studies of Oxygen Reduction by Hydrogen on PdAg(110). *ACS Catalysis*, **2013**, 3, 1622-1632	13.1	28
128	Atomic and molecular adsorption on Ru(0001). *Surface Science*, **2013**, 614, 64-74	1.8	62
127	Stabilization of copper catalysts for liquid-phase reactions by atomic layer deposition. *Angewandte Chemie - International Edition*, **2013**, 52, 13808-12	16.4	146
126	Stabilization of Copper Catalysts for Liquid-Phase Reactions by Atomic Layer Deposition. *Angewandte Chemie*, **2013**, 125, 14053-14057	3.6	39
125	Density Functional Theory and Reaction Kinetics Studies of the Water–Gas Shift Reaction on PtRe Catalysts. *ChemCatChem*, **2013**, 5, 3690-3699	5.2	25
124	Structure of Stoichiometric and Oxygen-Rich Ultrathin FeO(111) Films Grown on Pd(111). *Journal of Physical Chemistry C*, **2013**, 117, 15155-15163	3.8	43
123	Rücktitelbild: Stabilization of Copper Catalysts for Liquid-Phase Reactions by Atomic Layer Deposition (Angew. Chem. 51/2013). *Angewandte Chemie*, **2013**, 125, 14068-14068	3.6	1
122	Catalytic Activity of Platinum Monolayer on Iridium and Rhenium Alloy Nanoparticles for the Oxygen Reduction Reaction. *ACS Catalysis*, **2012**, 2, 817-824	13.1	84
121	Adsorbate-induced segregation in a PdAg membrane model system: Pd3Ag(1 1 1). *Catalysis Today*, **2012**, 193, 111-119	5.3	38

120	CO2 Hydrogenation to Formic Acid on Ni(111). *Journal of Physical Chemistry C*, **2012**, 116, 3001-3006	3.8	119
119	Hydrogen adsorption, absorption and diffusion on and in transition metal surfaces: A DFT study. *Surface Science*, **2012**, 606, 679-689	1.8	312
118	CO2 hydrogenation to formic acid on Ni(110). *Surface Science*, **2012**, 606, 1050-1055	1.8	64
117	Atomic and molecular adsorption on Pd(111). *Surface Science*, **2012**, 606, 1670-1679	1.8	88
116	Quantum tunneling enabled self-assembly of hydrogen atoms on Cu(111). *ACS Nano*, **2012**, 6, 10115-21	16.7	37
115	Bifunctional anode catalysts for direct methanol fuel cells. *Energy and Environmental Science*, **2012**, 5, 8335	35.4	138
114	A conversation with Haldor Topsø by Manos Mavrikakis. *Annual Review of Chemical and Biomolecular Engineering*, **2012**, 3, 1-10	8.9	5
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