Jean-Sabin McEwen

List of Publications by Year
in descending order

103 papers	4,654 citations	136950 32 h-index	102487 66 g-index
104 all docs	104 docs citations	104 times ranked	5312 citing authors

#	Article	IF	Citations
1	Carbon-supported bimetallic Pdâ€“Fe catalysts for vapor-phase hydrodeoxygenation of guaiacol. Journal of Catalysis, 2013, 306, 47-57.	6.2	384
2	Improving the deconvolution and interpretation of XPS spectra from chars by ab initio calculations. Carbon, 2016, 110, 155-171.	10.3	351
3	Deconvoluting the XPS spectra for nitrogen-doped chars: An analysis from first principles. Carbon, 2020, 162, 528-544.	10.3	323
4	An atomic-scale view of single-site Pt catalysis for low-temperature CO oxidation. Nature Catalysis, 2018, 1, 192-198.	34.4	292
5	Structural analysis of char by Raman spectroscopy: Improving band assignments through computational calculations from first principles. Carbon, 2016, 100, 678-692.	10.3	288
6	Elucidating the Roles of Electric Fields in Catalysis: A Perspective. ACS Catalysis, 2018, 8, 5153-5174.	11.2	215
7	Integrated operando X-ray absorption and DFT characterization of Cuâ€“SSZ-13 exchange sites during the selective catalytic reduction of NO with NH3. Catalysis Today, 2012, 184, 129-144.	4.4	212
8	Synergistic Catalysis between Pd and Fe in Gas Phase Hydrodeoxygenation of m-Cresol. ACS Catalysis, 2014, 4, 3335-3345.	11.2	173
9	NO Chemisorption on Cu/SSZ-13: A Comparative Study from Infrared Spectroscopy and DFT Calculations. ACS Catalysis, 2014, 4, 4093-4105.	11.2	139
10	Phenol Deoxygenation Mechanisms on Fe(110) and Pd(111). ACS Catalysis, 2015, 5, 523-536.	11.2	116
11	Enhanced Fe₂O₃ Reducibility via Surface Modification with Pd: Characterizing the Synergy within Pd/Fe Catalysts for Hydrodeoxygenation Reactions. ACS Catalysis, 2014, 4, 3381-3392.	11.2	114
12	Adsorption and desorption of CO on Pt(111): a comprehensive analysis. Surface Science, 2003, 545, 47-69.	1.9	99
13	DFT-Based Method for More Accurate Adsorption Energies: An Adaptive Sum of Energies from RPBE and vdW Density Functionals. Journal of Physical Chemistry C, 2017, 121, 4937-4945.	3.1	80
14	Improving Ni Catalysts Using Electric Fields: A DFT and Experimental Study of the Methane Steam Reforming Reaction. ACS Catalysis, 2017, 7, 551-562.	11.2	73
15	Improving the electrochemical oxidation of formic acid by tuning the electronic properties of Pd-based bimetallic nanoparticles. Applied Catalysis B: Environmental, 2019, 254, 685-692.	20.2	73
16	Probing Active-Site Relocation in Cu/SSZ-13 SCR Catalysts during Hydrothermal Aging by In Situ EPR Spectroscopy, Kinetics Studies, and DFT Calculations. ACS Catalysis, 2020, 10, 9410-9419.	11.2	64
17	Adsorption and desorption of CO on Ru(0001): A comprehensive analysis. Surface Science, 2005, 594, 240-262.	1.9	52
18	Adsorption of phenol on Fe (110) and Pd (111) from first principles. Surface Science, 2014, 630, 244-253.	1.9	52

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19	Catalytic water dehydrogenation and formation on nickel: Dual path mechanism in high electric fields. Journal of Catalysis, 2015, 332, 187-200.	6.2	52
20	Microstructural analysis of nitrogen-doped char by Raman spectroscopy: Raman shift analysis from first principles. Carbon, 2020, 167, 559-574.	10.3	52
21	Nanometric chemical clocks. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 3006-3010.	7.1	50
22	How low can you go? Minimum energy pathways for O2 dissociation on Pt(111). Physical Chemistry Chemical Physics, 2012, 14, 16677.	2.8	50
23	Mechanistic Effects of Water on the Fe-Catalyzed Hydrodeoxygenation of Phenol. The Role of BrÃ¸nsted Acid Sites. ACS Catalysis, 2018, 8, 2200-2208.	11.2	50
24	Oscillations and Bistability in the Catalytic Formation of Water on Rhodium in High Electric Fields. Journal of Physical Chemistry C, 2009, 113, 17045-17058.	3.1	45
25	Tailoring the Adsorption of Benzene on PdFe Surfaces: A Density Functional Theory Study. Journal of Physical Chemistry C, 2013, 117, 24317-24328.	3.1	45
26	Structurally Accurate Model for the â€œ29â€•Structure of Cu_xO/Cu(111): A DFT and STM Study. Journal of Physical Chemistry C, 2016, 120, 10879-10886.	3.1	45
27	Elucidating the field influence on the energetics of the methane steam reforming reaction: A density functional theory study. Applied Catalysis B: Environmental, 2016, 195, 77-89.	20.2	45
28	Perspective on Catalytic Hydrodeoxygenation of Biomass Pyrolysis Oils: Essential Roles of Fe-Based Catalysts. Catalysis Letters, 2016, 146, 1621-1633.	2.6	42
29	Catalytic Reaction Rates Controlled by Metal Oxidation State: Câ^'H Bond Cleavage in Methane over Nickelâ€Based Catalysts. Angewandte Chemie - International Edition, 2017, 56, 3557-3561.	13.8	39
30	Adsorption of guaiacol on Fe (110) and Pd (111) from first principles. Surface Science, 2016, 648, 227-235.	1.9	36
31	Local Environment Sensitivity of the Cu K-Edge XANES Features in Cu-SSZ-13: Analysis from First-Principles. Journal of Physical Chemistry Letters, 2018, 9, 3035-3042.	4.6	34
32	Accelerated Cu₂O Reduction by Single Pt Atoms at the Metal-Oxide Interface. ACS Catalysis, 2020, 10, 4215-4226.	11.2	34
33	Controlling the Oxidation State of Fe-Based Catalysts through Nitrogen Doping toward the Hydrodeoxygenation of m-Cresol. ACS Catalysis, 2020, 10, 7884-7893.	11.2	32
34	Density functional theory studies of methyl dissociation on a Ni(111) surface in the presence of an external electric field. Physical Chemistry Chemical Physics, 2014, 16, 2399-2410.	2.8	31
35	CO-induced inversion of the layer sequence of a model CoCu catalyst. Surface Science, 2016, 648, 74-83.	1.9	30
36	Reducing Reaction Temperature, Steam Requirements, and Coke Formation During Methane Steam Reforming Using Electric Fields: A Microkinetic Modeling and Experimental Study. ACS Catalysis, 2017, 7, 6957-6968.	11.2	30

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37	Decomposition of methyl species on a Ni(211) surface: investigations of the electric field influence. Catalysis Science and Technology, 2014, 4, 4020-4035.	4.1	29
38	The Role of Protons and Hydrides in the Catalytic Hydrogenolysis of Guaiacol at the Ruthenium Nanoparticleâ€“Water Interface. ACS Catalysis, 2020, 10, 12310-12332.	11.2	29
39	Mechanistic understanding of methanol carbonylation: Interfacing homogeneous and heterogeneous catalysis via carbon supported Ir La. Journal of Catalysis, 2018, 361, 414-422.	6.2	28
40	Field-assisted oxidation of rhodium. Chemical Physics Letters, 2008, 452, 133-138.	2.6	26
41	Integrated X-ray photoelectron spectroscopy and DFT characterization of benzene adsorption on Pt(111), Pt(355) and Pt(322) surfaces. Physical Chemistry Chemical Physics, 2013, 15, 20662.	2.8	25
42	First-principles reaction site model for coverage-sensitive surface reactions: Pt(111)â€“O temperature programmed desorption. Surface Science, 2014, 622, L1-L6.	1.9	24
43	CO Adsorption on the â€œ29â€•Cu_xO/Cu(111) Surface: An Integrated DFT, STM, and TPD Study. Journal of Physical Chemistry C, 2016, 120, 25387-25394.	3.1	24
44	Enhancing the partial oxidation of gasoline with Mo-doped Ni catalysts for SOFC applications: An integrated experimental and DFT study. Applied Catalysis B: Environmental, 2020, 266, 118626.	20.2	24
45	Phase diagram of O/Ru(0001) from first principles. Chemical Physics Letters, 2002, 361, 317-320.	2.6	23
46	The interaction of reactants, intermediates and products with Cu ions in Cu-SSZ-13 NH₃SCR catalysts: an energetic and ab initio X-ray absorption modeling study. Catalysis Science and Technology, 2016, 6, 5812-5829.	4.1	23
47	Unravelling the reaction mechanism of gas-phase formic acid decomposition on highly dispersed Mo2C nanoparticles supported on graphene flakes. Applied Catalysis B: Environmental, 2020, 264, 118478.	20.2	23
48	Electric field induced oscillations in the catalytic water production on rhodium: A theoretical analysis. Surface Science, 2010, 604, 1353-1368.	1.9	22
49	Effect of pyrolysis temperature on aromatic cluster size of cellulose char by quantitative multi cross-polarization 13C NMR with long range dipolar dephasing. Carbon, 2017, 116, 210-222.	10.3	22
50	Thermodynamic stability of nitrogen functionalities and defects in graphene and graphene nanoribbons from first principles. Carbon, 2019, 152, 715-726.	10.3	22
51	Catalytic Reduction of NO₂with Hydrogen on Pt Field Emitter Tips: Kinetic Instabilities on the Nanoscale. Langmuir, 2010, 26, 16381-16391.	3.5	20
52	Role of Carbon Monoxide in Catalyst Reconstruction for CO Hydrogenation: First-Principles Study of the Composition, Structure, and Stability of Cu/Co(101Ì…2) as a Function of CO Pressure. Journal of Physical Chemistry C, 2017, 121, 2181-2191.	3.1	20
53	Field-assisted suppression of coke in the methane steam reforming reaction. Applied Catalysis B: Environmental, 2020, 260, 118132.	20.2	20
54	Chemisorption-Induced Formation of Biphenylene Dimer on Ag(111). Journal of the American Chemical Society, 2022, 144, 723-732.	13.7	20

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55	Developing single-site Pt catalysts for the preferential oxidation of CO: A surface science and first principles-guided approach. Applied Catalysis B: Environmental, 2021, 284, 119716.	20.2	19
56	Water activation by single Pt atoms supported on a Cu2O thin film. Journal of Catalysis, 2018, 364, 166-173.	6.2	18
57	Catalytic Reaction Rates Controlled by Metal Oxidation State: Câ^'H Bond Cleavage in Methane over Nickelâ€Based Catalysts. Angewandte Chemie, 2017, 129, 3611-3615.	2.0	16
58	Modeling the Adsorption of NO and NH₃ on Fe-SSZ-13 from First-Principles: A DFT Study. Industrial & Engineering Chemistry Research, 2018, 57, 13396-13405.	3.7	16
59	Coverage-Dependent Adsorption of Hydrogen on Fe(100): Determining Catalytically Relevant Surface Structures via Lattice Gas Models. Journal of Physical Chemistry C, 2020, 124, 7254-7266.	3.1	15
60	Catalytic consequences of hydrogen addition events and solvent-adsorbate interactions during guaiacol-H2 reactions at the H2O-Ru(0Â0Â0Â1) interface. Journal of Catalysis, 2021, 395, 467-482.	6.2	15
61	Non-equilibrium surface pattern formation during catalytic reactions with nanoscale resolution: Investigations of the electric field influence. Catalysis Today, 2010, 154, 75-84.	4.4	14
62	Adsorption of aromatics on the (111) surface of PtM and PtM₃ (M = Fe, Ni) alloys. RSC Advances, 2015, 5, 85705-85719.	3.6	14
63	Hydrogen Oxidation and Water Dissociation over an Oxygen-Enriched Ni/YSZ Electrode in the Presence of an Electric Field: A First-Principles-Based Microkinetic Model. Industrial & Engineering Chemistry Research, 2017, 56, 1201-1213.	3.7	13
64	Elucidating the Role of the Electric Field at the Ni/YSZ Electrode: A DFT Study. Journal of Physical Chemistry C, 2016, 120, 14608-14620.	3.1	12
65	Chemical Sensitivity of Valence-to-Core X-ray Emission Spectroscopy Due to the Ligand and the Oxidation State: A Computational Study on Cu-SSZ-13 with Multiple H₂O and NH₃ Adsorption. Journal of Physical Chemistry C, 2017, 121, 25759-25767.	3.1	12
66	Coverage-Dependent Adsorption of Phenol on Pt(111) from First Principles. Journal of Physical Chemistry C, 2020, 124, 356-362.	3.1	12
67	CO oxidation on electrically charged gold nanotips. Journal of Chemical Physics, 2006, 125, 214707.	3.0	11
68	Dissolution of CoCu catalyst step defects by Co subcarbonyl formation. Journal of Catalysis, 2018, 368, 31-37.	6.2	11
69	Predicting the Electric Field Effect on the Lateral Interactions Between Adsorbates: O/Fe(100) from First Principles. Topics in Catalysis, 2018, 61, 763-775.	2.8	11
70	Enhancing Chemical Interaction of Polysulfide and Carbon through Synergetic Nitrogen and Phosphorus Doping. ACS Sustainable Chemistry and Engineering, 2020, 8, 806-813.	6.7	11
71	Ab initio X-ray absorption modeling of Cu-SAPO-34: Characterization of Cu exchange sites under different conditions. Catalysis Today, 2016, 267, 28-40.	4.4	10
72	Characterization of CoCu- and CoMn-Based Catalysts for the Fischerâ€“Tropsch Reaction Toward Chain-Lengthened Oxygenates. Topics in Catalysis, 2018, 61, 1016-1023.	2.8	10

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73	Benchmarking the accuracy of coverage-dependent models: adsorption and desorption of benzene on Pt (1â€¯1â€¯1) and Pt3Sn (1â€¯1â€¯1) from first principles. Progress in Surface Science, 2019, 94, 100538.	8.3	10
74	Formulation of Multicomponent Lattice Gas Model Cluster Expansions Parameterized on Ab Initio Data: An Introduction to the Ab Initio Mean-Field Augmented Lattice Gas Modeling Code. Journal of Physical Chemistry C, 2020, 124, 2923-2938.	3.1	10
75	Characterizing the geometric and electronic structure of defects in the â€œ29â€•copper surface oxide. Journal of Chemical Physics, 2017, 147, 224706.	3.0	9
76	Controlling Molecular Switching via Chemical Functionality: Ethyl vs Methoxy Rotors. Journal of Physical Chemistry C, 2019, 123, 23738-23746.	3.1	9
77	Surface-Templated Assembly of Molecular Methanol on the Thin Film â€œ29â€•Cu(111) Surface Oxide. Journal of Physical Chemistry C, 2019, 123, 2911-2921.	3.1	9
78	Lateral interactions and nonequilibrium in adsorption and desorption. Part 2. A kinetic lattice gas model for (2Ã—2)-(3O+NO)/Ru(001). Surface Science, 2006, 600, 4660-4669.	1.9	8
79	Understanding Enantioselective Interactions by Pulling Apart Molecular Rotor Complexes. ACS Nano, 2019, 13, 5939-5946.	14.6	8
80	Promoting the Cleavage of Câ€“O Bonds at the Interface between a Metal Oxide Cluster and a Co(0001) Support. ACS Catalysis, 2020, 10, 14722-14731.	11.2	8
81	Elucidating the Role of B-Site Cations toward CO₂ Reduction in Perovskite-Based Solid Oxide Electrolysis Cells. Journal of the Electrochemical Society, 2022, 169, 034532.	2.9	8
82	Two-Dimensional Roughening of Adsorbate Islands in Thermodynamic Equilibrium. Physical Review Letters, 2006, 96, 166102.	7.8	7
83	The partial reduction of clean and doped Î±-Fe2O3(0001) from first principles. Applied Catalysis A: General, 2019, 582, 116989.	4.3	6
84	Hopping kinetics on a finite 1D chain: An exact analysis. International Journal of Quantum Chemistry, 2006, 106, 2889-2903.	2.0	5
85	Identifying the Thermal Decomposition Mechanism of Guaiacol on Pt(111): An Integrated X-ray Photoelectron Spectroscopy and Density Functional Theory Study. Journal of Physical Chemistry C, 2018, 122, 4261-4273.	3.1	5
86	Templated Growth of a Homochiral Thin Film Oxide. ACS Nano, 2020, 14, 4682-4688.	14.6	5
87	Elucidating the Influence of Electric Fields toward CO2 Activation on YSZ (111). Catalysts, 2021, 11, 271.	3.5	5
88	Elucidating the Cooperative Roles of Water and Lewis Acidâ€“Base Pairs in Cascade Câ€“C Coupling and Self-Deoxygenation Reactions. Jacs Au, 2021, 1, 1471-1487.	7.9	5
89	First-Principles Approach to Extracting Chemical Information from X-ray Absorption Near-Edge Spectra of Ga-Containing Materials. Journal of Physical Chemistry C, 2021, 125, 27901-27908.	3.1	5
90	Modeling the adsorbate coverage distribution over a multi-faceted catalytic grain in the presence of an electric field: O/Fe from first principles. Catalysis Today, 2018, 312, 92-104.	4.4	4

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91	Nitrogen-doped char as a catalyst for wet oxidation of phenol-contaminated water. Biomass Conversion and Biorefinery, 2024, 14, 5861-5875.	4.6	4
92	Visualizing the origin of rotational entropy effects in coadsorbed systems. Physical Review Research, 2020, 2, .	3.6	4
93	Determining the hydration energetics on carbon-supported Ru catalysts: An adsorption calorimetry and density functional theory study. Catalysis Today, 2021, 365, 172-180.	4.4	3
94	Guiding the design of oxidation-resistant Fe-based single atom alloy catalysts with insights from configurational space. Journal of Chemical Physics, 2021, 154, 174709.	3.0	3
95	BrÃ¸nsted acidity of H-adatoms at protic solvent-transition metal interfaces and its kinetic consequences in electrophilic addition reactions. Journal of Catalysis, 2022, 408, 179-195.	6.2	3
96	Quantifying Errors in Effective Cluster Interactions of Lattice Gas Cluster Expansions. Journal of Physical Chemistry C, 0, , .	3.1	2
97	Microscopic insights into long-range 1D ordering in a dense semi-disordered molecular overlayer. Chemical Communications, 2021, 57, 5937-5940.	4.1	1
98	Novel Amorphous Carbons for the Adsorption of Phosphate: Part I. Elucidation of Chemical Structure of N-Metal-Doped Chars. ACS Omega, 2022, 7, 14490-14504.	3.5	1
99	Elucidating CO Oxidation Pathways on Rh Atoms and Clusters on the â€œ29â€•Cu₂O/Cu(111) Surface. Journal of Physical Chemistry C, 2022, 126, 11091-11102.	3.1	1
100	InnenrÃ¼cktitelbild: Catalytic Reaction Rates Controlled by Metal Oxidation State: Câ^'H Bond Cleavage in Methane over Nickelâ€Based Catalysts (Angew. Chem. 13/2017). Angewandte Chemie, 2017, 129, 3777-3777.	2.0	0
101	Computational Catalysis at NAM25. Catalysis Today, 2018, 312, 1.	4.4	0
102	Identifying Trends in the Field Ionization of Diatomic Molecules over Adsorbate Covered Pd(331) Surfaces. Topics in Catalysis, 2020, 63, 1510-1521.	2.8	0
103	Determining the Adsorption Energetics of 2,3-Butanediol on RuO2(110): Coupling First-Principles Calculations With Global Optimizers. Frontiers in Energy Research, 2022, 9, .	2.3	0