

Jean-Sabin McEwen

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7627271/publications.pdf>

Version: 2024-02-01

103
papers

4,654
citations

136940

32
h-index

102480

66
g-index

104
all docs

104
docs citations

104
times ranked

5312
citing authors

#	ARTICLE	IF	CITATIONS
1	Carbon-supported bimetallic Pd-Fe catalysts for vapor-phase hydrodeoxygenation of guaiacol. <i>Journal of Catalysis</i> , 2013, 306, 47-57.	6.2	384
2	Improving the deconvolution and interpretation of XPS spectra from chars by ab initio calculations. <i>Carbon</i> , 2016, 110, 155-171.	10.3	351
3	Deconvoluting the XPS spectra for nitrogen-doped chars: An analysis from first principles. <i>Carbon</i> , 2020, 162, 528-544.	10.3	323
4	An atomic-scale view of single-site Pt catalysis for low-temperature CO oxidation. <i>Nature Catalysis</i> , 2018, 1, 192-198.	34.4	292
5	Structural analysis of char by Raman spectroscopy: Improving band assignments through computational calculations from first principles. <i>Carbon</i> , 2016, 100, 678-692.	10.3	288
6	Elucidating the Roles of Electric Fields in Catalysis: A Perspective. <i>ACS Catalysis</i> , 2018, 8, 5153-5174.	11.2	215
7	Integrated operando X-ray absorption and DFT characterization of Cu-SSZ-13 exchange sites during the selective catalytic reduction of NO with NH ₃ . <i>Catalysis Today</i> , 2012, 184, 129-144.	4.4	212
8	Synergistic Catalysis between Pd and Fe in Gas Phase Hydrodeoxygenation of <i>m</i> -Cresol. <i>ACS Catalysis</i> , 2014, 4, 3335-3345.	11.2	173
9	NO Chemisorption on Cu/SSZ-13: A Comparative Study from Infrared Spectroscopy and DFT Calculations. <i>ACS Catalysis</i> , 2014, 4, 4093-4105.	11.2	139
10	Phenol Deoxygenation Mechanisms on Fe(110) and Pd(111). <i>ACS Catalysis</i> , 2015, 5, 523-536.	11.2	116
11	Enhanced Fe ₂ O ₃ Reducibility via Surface Modification with Pd: Characterizing the Synergy within Pd/Fe Catalysts for Hydrodeoxygenation Reactions. <i>ACS Catalysis</i> , 2014, 4, 3381-3392.	11.2	114
12	Adsorption and desorption of CO on Pt(111): a comprehensive analysis. <i>Surface Science</i> , 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. <i>Journal of Physical Chemistry C</i> , 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. <i>ACS Catalysis</i> , 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. <i>Applied Catalysis B: Environmental</i> , 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. <i>ACS Catalysis</i> , 2020, 10, 9410-9419.	11.2	64
17	Adsorption and desorption of CO on Ru(0001): A comprehensive analysis. <i>Surface Science</i> , 2005, 594, 240-262.	1.9	52
18	Adsorption of phenol on Fe (110) and Pd (111) from first principles. <i>Surface Science</i> , 2014, 630, 244-253.	1.9	52

#	ARTICLE	IF	CITATIONS
19	Catalytic water dehydrogenation and formation on nickel: Dual path mechanism in high electric fields. <i>Journal of Catalysis</i> , 2015, 332, 187-200.	6.2	52
20	Microstructural analysis of nitrogen-doped char by Raman spectroscopy: Raman shift analysis from first principles. <i>Carbon</i> , 2020, 167, 559-574.	10.3	52
21	Nanometric chemical clocks. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 3006-3010.	7.1	50
22	How low can you go? Minimum energy pathways for O ₂ dissociation on Pt(111). <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16677.	2.8	50
23	Mechanistic Effects of Water on the Fe-Catalyzed Hydrodeoxygenation of Phenol. The Role of Brønsted Acid Sites. <i>ACS Catalysis</i> , 2018, 8, 2200-2208.	11.2	50
24	Oscillations and Bistability in the Catalytic Formation of Water on Rhodium in High Electric Fields. <i>Journal of Physical Chemistry C</i> , 2009, 113, 17045-17058.	3.1	45
25	Tailoring the Adsorption of Benzene on PdFe Surfaces: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24317-24328.	3.1	45
26	Structurally Accurate Model for the α -Structure of Cu ₂ O/Cu(111): A DFT and STM Study. <i>Journal of Physical Chemistry C</i> , 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. <i>Applied Catalysis B: Environmental</i> , 2016, 195, 77-89.	20.2	45
28	Perspective on Catalytic Hydrodeoxygenation of Biomass Pyrolysis Oils: Essential Roles of Fe-Based Catalysts. <i>Catalysis Letters</i> , 2016, 146, 1621-1633.	2.6	42
29	Catalytic Reaction Rates Controlled by Metal Oxidation State: C-H Bond Cleavage in Methane over Nickel-Based Catalysts. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 3557-3561.	13.8	39
30	Adsorption of guaiacol on Fe (110) and Pd (111) from first principles. <i>Surface Science</i> , 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. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3035-3042.	4.6	34
32	Accelerated Cu ₂ O Reduction by Single Pt Atoms at the Metal-Oxide Interface. <i>ACS Catalysis</i> , 2020, 10, 4215-4226.	11.2	34
33	Controlling the Oxidation State of Fe-Based Catalysts through Nitrogen Doping toward the Hydrodeoxygenation of <i>m</i> -Cresol. <i>ACS Catalysis</i> , 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. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2399-2410.	2.8	31
35	CO-induced inversion of the layer sequence of a model CoCu catalyst. <i>Surface Science</i> , 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. <i>ACS Catalysis</i> , 2017, 7, 6957-6968.	11.2	30

#	ARTICLE	IF	CITATIONS
37	Decomposition of methyl species on a Ni(211) surface: investigations of the electric field influence. <i>Catalysis Science and Technology</i> , 2014, 4, 4020-4035.	4.1	29
38	The Role of Protons and Hydrides in the Catalytic Hydrogenolysis of Guaiacol at the Ruthenium Nanoparticle-Water Interface. <i>ACS Catalysis</i> , 2020, 10, 12310-12332.	11.2	29
39	Mechanistic understanding of methanol carbonylation: Interfacing homogeneous and heterogeneous catalysis via carbon supported Ir La. <i>Journal of Catalysis</i> , 2018, 361, 414-422.	6.2	28
40	Field-assisted oxidation of rhodium. <i>Chemical Physics Letters</i> , 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. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20662.	2.8	25
42	First-principles reaction site model for coverage-sensitive surface reactions: Pt(111)-O temperature programmed desorption. <i>Surface Science</i> , 2014, 622, L1-L6.	1.9	24
43	CO Adsorption on the $\text{Cu}/\text{Cu}(\text{111})$ Surface: An Integrated DFT, STM, and TPD Study. <i>Journal of Physical Chemistry C</i> , 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. <i>Applied Catalysis B: Environmental</i> , 2020, 266, 118626.	20.2	24
45	Phase diagram of O/Ru(0001) from first principles. <i>Chemical Physics Letters</i> , 2002, 361, 317-320.	2.6	23
46	The interaction of reactants, intermediates and products with Cu ions in Cu-SSZ-13 NH_3 SCR catalysts: an energetic and ab initio X-ray absorption modeling study. <i>Catalysis Science and Technology</i> , 2016, 6, 5812-5829.	4.1	23
47	Unravelling the reaction mechanism of gas-phase formic acid decomposition on highly dispersed Mo ₂ C nanoparticles supported on graphene flakes. <i>Applied Catalysis B: Environmental</i> , 2020, 264, 118478.	20.2	23
48	Electric field induced oscillations in the catalytic water production on rhodium: A theoretical analysis. <i>Surface Science</i> , 2010, 604, 1353-1368.	1.9	22
49	Effect of pyrolysis temperature on aromatic cluster size of cellulose char by quantitative multi cross-polarization ¹³ C NMR with long range dipolar dephasing. <i>Carbon</i> , 2017, 116, 210-222.	10.3	22
50	Thermodynamic stability of nitrogen functionalities and defects in graphene and graphene nanoribbons from first principles. <i>Carbon</i> , 2019, 152, 715-726.	10.3	22
51	Catalytic Reduction of NO ₂ with Hydrogen on Pt Field Emitter Tips: Kinetic Instabilities on the Nanoscale. <i>Langmuir</i> , 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(101...2) as a Function of CO Pressure. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2181-2191.	3.1	20
53	Field-assisted suppression of coke in the methane steam reforming reaction. <i>Applied Catalysis B: Environmental</i> , 2020, 260, 118132.	20.2	20
54	Chemisorption-Induced Formation of Biphenylene Dimer on Ag(111). <i>Journal of the American Chemical Society</i> , 2022, 144, 723-732.	13.7	20

#	ARTICLE	IF	CITATIONS
55	Developing single-site Pt catalysts for the preferential oxidation of CO: A surface science and first principles-guided approach. <i>Applied Catalysis B: Environmental</i> , 2021, 284, 119716.	20.2	19
56	Water activation by single Pt atoms supported on a Cu ₂ O thin film. <i>Journal of Catalysis</i> , 2018, 364, 166-173.	6.2	18
57	Catalytic Reaction Rates Controlled by Metal Oxidation State: C-H Bond Cleavage in Methane over Nickel-Based Catalysts. <i>Angewandte Chemie</i> , 2017, 129, 3611-3615.	2.0	16
58	Modeling the Adsorption of NO and NH ₃ on Fe-SSZ-13 from First-Principles: A DFT Study. <i>Industrial & Engineering Chemistry Research</i> , 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. <i>Journal of Physical Chemistry C</i> , 2020, 124, 7254-7266.	3.1	15
60	Catalytic consequences of hydrogen addition events and solvent-adsorbate interactions during guaiacol-H ₂ reactions at the H ₂ O-Ru(O) interface. <i>Journal of Catalysis</i> , 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. <i>Catalysis Today</i> , 2010, 154, 75-84.	4.4	14
62	Adsorption of aromatics on the (111) surface of PtM and PtM ₃ (M = Fe, Ni) alloys. <i>RSC Advances</i> , 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. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 1201-1213.	3.7	13
64	Elucidating the Role of the Electric Field at the Ni/YSZ Electrode: A DFT Study. <i>Journal of Physical Chemistry C</i> , 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 H ₂ O and NH ₃ Adsorption. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25759-25767.	3.1	12
66	Coverage-Dependent Adsorption of Phenol on Pt(111) from First Principles. <i>Journal of Physical Chemistry C</i> , 2020, 124, 356-362.	3.1	12
67	CO oxidation on electrically charged gold nanotips. <i>Journal of Chemical Physics</i> , 2006, 125, 214707.	3.0	11
68	Dissolution of CoCu catalyst step defects by Co subcarbonyl formation. <i>Journal of Catalysis</i> , 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. <i>Topics in Catalysis</i> , 2018, 61, 763-775.	2.8	11
70	Enhancing Chemical Interaction of Polysulfide and Carbon through Synergetic Nitrogen and Phosphorus Doping. <i>ACS Sustainable Chemistry and Engineering</i> , 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. <i>Catalysis Today</i> , 2016, 267, 28-40.	4.4	10
72	Characterization of CoCu- and CoMn-Based Catalysts for the Fischer-Tropsch Reaction Toward Chain-Lengthened Oxygenates. <i>Topics in Catalysis</i> , 2018, 61, 1016-1023.	2.8	10

#	ARTICLE	IF	CITATIONS
73	Benchmarking the accuracy of coverage-dependent models: adsorption and desorption of benzene on Pt (111) and Pt ₃ Sn (111) from first principles. <i>Progress in Surface Science</i> , 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. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2923-2938.	3.1	10
75	Characterizing the geometric and electronic structure of defects in the α -copper surface oxide. <i>Journal of Chemical Physics</i> , 2017, 147, 224706.	3.0	9
76	Controlling Molecular Switching via Chemical Functionality: Ethyl vs Methoxy Rotors. <i>Journal of Physical Chemistry C</i> , 2019, 123, 23738-23746.	3.1	9
77	Surface-Templated Assembly of Molecular Methanol on the Thin Film α -Cu(111) Surface Oxide. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2911-2921.	3.1	9
78	Lateral interactions and nonequilibrium in adsorption and desorption. Part 2. A kinetic lattice gas model for (2 \times 2)-(3O+NO)/Ru(001). <i>Surface Science</i> , 2006, 600, 4660-4669.	1.9	8
79	Understanding Enantioselective Interactions by Pulling Apart Molecular Rotor Complexes. <i>ACS Nano</i> , 2019, 13, 5939-5946.	14.6	8
80	Promoting the Cleavage of C=O Bonds at the Interface between a Metal Oxide Cluster and a Co(0001) Support. <i>ACS Catalysis</i> , 2020, 10, 14722-14731.	11.2	8
81	Elucidating the Role of B-Site Cations toward CO ₂ Reduction in Perovskite-Based Solid Oxide Electrolysis Cells. <i>Journal of the Electrochemical Society</i> , 2022, 169, 034532.	2.9	8
82	Two-Dimensional Roughening of Adsorbate Islands in Thermodynamic Equilibrium. <i>Physical Review Letters</i> , 2006, 96, 166102.	7.8	7
83	The partial reduction of clean and doped γ -Fe ₂ O ₃ (0001) from first principles. <i>Applied Catalysis A: General</i> , 2019, 582, 116989.	4.3	6
84	Hopping kinetics on a finite 1D chain: An exact analysis. <i>International Journal of Quantum Chemistry</i> , 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. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4261-4273.	3.1	5
86	Templated Growth of a Homochiral Thin Film Oxide. <i>ACS Nano</i> , 2020, 14, 4682-4688.	14.6	5
87	Elucidating the Influence of Electric Fields toward CO ₂ Activation on YSZ (111). <i>Catalysts</i> , 2021, 11, 271.	3.5	5
88	Elucidating the Cooperative Roles of Water and Lewis Acid-Base Pairs in Cascade C-C Coupling and Self-Deoxygenation Reactions. <i>Jacs Au</i> , 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. <i>Journal of Physical Chemistry C</i> , 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. <i>Catalysis Today</i> , 2018, 312, 92-104.	4.4	4

#	ARTICLE	IF	CITATIONS
91	Nitrogen-doped char as a catalyst for wet oxidation of phenol-contaminated water. <i>Biomass Conversion and Biorefinery</i> , 2024, 14, 5861-5875.	4.6	4
92	Visualizing the origin of rotational entropy effects in coadsorbed systems. <i>Physical Review Research</i> , 2020, 2, .	3.6	4
93	Determining the hydration energetics on carbon-supported Ru catalysts: An adsorption calorimetry and density functional theory study. <i>Catalysis Today</i> , 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. <i>Journal of Chemical Physics</i> , 2021, 154, 174709.	3.0	3
95	Brønsted acidity of H-adatoms at protic solvent-transition metal interfaces and its kinetic consequences in electrophilic addition reactions. <i>Journal of Catalysis</i> , 2022, 408, 179-195.	6.2	3
96	Quantifying Errors in Effective Cluster Interactions of Lattice Gas Cluster Expansions. <i>Journal of Physical Chemistry C</i> , 0, , .	3.1	2
97	Microscopic insights into long-range 1D ordering in a dense semi-disordered molecular overlayer. <i>Chemical Communications</i> , 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. <i>ACS Omega</i> , 2022, 7, 14490-14504.	3.5	1
99	Elucidating CO Oxidation Pathways on Rh Atoms and Clusters on the $\alpha\text{-Cu}_2\text{O}/\text{Cu}(111)$ Surface. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11091-11102.	3.1	1
100	Innenrücktitelbild: Catalytic Reaction Rates Controlled by Metal Oxidation State: C-H Bond Cleavage in Methane over Nickel-Based Catalysts (<i>Angew. Chem.</i> 13/2017). <i>Angewandte Chemie</i> , 2017, 129, 3777-3777.	2.0	0
101	Computational Catalysis at NAM25. <i>Catalysis Today</i> , 2018, 312, 1.	4.4	0
102	Identifying Trends in the Field Ionization of Diatomic Molecules over Adsorbate Covered Pd(331) Surfaces. <i>Topics in Catalysis</i> , 2020, 63, 1510-1521.	2.8	0
103	Determining the Adsorption Energetics of 2,3-Butanediol on RuO ₂ (110): Coupling First-Principles Calculations With Global Optimizers. <i>Frontiers in Energy Research</i> , 2022, 9, .	2.3	0