David D Hibbitts

List of Publications by Year
in descending order

45 papers	3,217 citations	186209 28 h-index	223716 46 g-index
52 all docs	52 docs citations	52 times ranked	3801 citing authors

#	Article	IF	Citations
1	Reactivity of the Gold/Water Interface During Selective Oxidation Catalysis. Science, 2010, 330, 74-78.	6.0	888
2	Selective Hydrogenolysis of Polyols and Cyclic Ethers over Bifunctional Surface Sites on Rhodiumâ€“Rhenium Catalysts. Journal of the American Chemical Society, 2011, 133, 12675-12689.	6.6	439
3	Interfacial charge distributions in carbon-supported palladium catalysts. Nature Communications, 2017, 8, 340.	5.8	145
4	Mechanistic Role of Water on the Rate and Selectivity of Fischerâ€“Tropsch Synthesis on Ruthenium Catalysts. Angewandte Chemie - International Edition, 2013, 52, 12273-12278.	7.2	138
5	Electrocatalysis: A direct alcohol fuel cell and surface science perspective. Catalysis Today, 2013, 202, 197-209.	2.2	130
6	Metal-Catalyzed Câ€“C Bond Cleavage in Alkanes: Effects of Methyl Substitution on Transition-State Structures and Stability. Journal of the American Chemical Society, 2014, 136, 9664-9676.	6.6	87
7	Dominant Role of Entropy in Stabilizing Sugar Isomerization Transition States within Hydrophobic Zeolite Pores. Journal of the American Chemical Society, 2018, 140, 14244-14266.	6.6	83
8	Influence of oxygen and pH on the selective oxidation of ethanol on Pd catalysts. Journal of Catalysis, 2013, 299, 261-271.	3.1	63
9	Promotional effects of chemisorbed oxygen and hydroxide in the activation of Câ€“H and Oâ€“H bonds over transition metal surfaces. Surface Science, 2016, 650, 210-220.	0.8	57
10	Theoretical and kinetic assessment of the mechanism of ethane hydrogenolysis on metal surfaces saturated with chemisorbed hydrogen. Journal of Catalysis, 2014, 311, 350-356.	3.1	55
11	Kinetic and Mechanistic Assessment of Alkanol/Alkanal Decarbonylation and Deoxygenation Pathways on Metal Catalysts. Journal of the American Chemical Society, 2015, 137, 11984-11995.	6.6	55
12	Experimental and Theoretical Assessments of Aluminum Proximity in MFI Zeolites and Its Alteration by Organic and Inorganic Structure-Directing Agents. Chemistry of Materials, 2020, 32, 9277-9298.	3.2	55
13	Preferential activation of CO near hydrocarbon chains during Fischerâ€“Tropsch synthesis on Ru. Journal of Catalysis, 2016, 337, 91-101.	3.1	54
14	Dense CO Adlayers as Enablers of CO Hydrogenation Turnovers on Ru Surfaces. Journal of the American Chemical Society, 2017, 139, 11789-11802.	6.6	54
15	Prevalence of Bimolecular Routes in the Activation of Diatomic Molecules with Strong Chemical Bonds (O2, NO, CO, N2) on Catalytic Surfaces. Accounts of Chemical Research, 2015, 48, 1254-1262.	7.6	53
16	Effects of Chain Length on the Mechanism and Rates of Metal-Catalyzed Hydrogenolysis of n-Alkanes. Journal of Physical Chemistry C, 2016, 120, 8125-8138.	1.5	49
17	Mechanism and Kinetics of Methylating C₆â€“C₁₂ Methylbenzenes with Methanol and Dimethyl Ether in H-MFI Zeolites. ACS Catalysis, 2019, 9, 6444-6460.	5.5	45
18	Tuning BrÃ¸nsted Acid Strength by Altering Site Proximity in CHA Framework Zeolites. ACS Catalysis, 2018, 8, 7842-7860.	5.5	41

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19	Role of Branching on the Rate and Mechanism of Câ€“C Cleavage in Alkanes on Metal Surfaces. ACS Catalysis, 2016, 6, 469-482.	5.5	40
20	Mechanistic origins of the high-pressure inhibition of methanol dehydration rates in small-pore acidic zeolites. Journal of Catalysis, 2019, 380, 161-177.	3.1	40
21	Highly Selective Cross-Etherification of 5-Hydroxymethylfurfural with Ethanol. ACS Catalysis, 2020, 10, 6771-6785.	5.5	40
22	Acid strength and bifunctional catalytic behavior of alloys comprised of noble metals and oxophilic metal promoters. Journal of Catalysis, 2014, 315, 48-58.	3.1	39
23	Contrasting Arene, Alkene, Diene, and Formaldehyde Hydrogenation in H-ZSM-5, H-SSZ-13, and H-SAPO-34 Frameworks during MTO. ACS Catalysis, 2020, 10, 4593-4607.	5.5	38
24	Catalytic NO activation and NOâ€“H 2 reaction pathways. Journal of Catalysis, 2014, 319, 95-109.	3.1	31
25	Comparing Rate and Mechanism of Ethane Hydrogenolysis on Transition-Metal Catalysts. Journal of Physical Chemistry C, 2019, 123, 5421-5432.	1.5	31
26	In Situ Methods for Identifying Reactive Surface Intermediates during Hydrogenolysis Reactions: Câ€“O Bond Cleavage on Nanoparticles of Nickel and Nickel Phosphides. Journal of the American Chemical Society, 2019, 141, 16671-16684.	6.6	30
27	Mechanisms and Active Sites for Câ€“O Bond Rupture within 2-Methyltetrahydrofuran over Ni, Ni₁₂P₅, and Ni₂P Catalysts. ACS Catalysis, 2018, 8, 7141-7157.	5.5	29
28	Rigid Arrangements of Ionic Charge in Zeolite Frameworks Conferred by Specific Aluminum Distributions Preferentially Stabilize Alkanol Dehydration Transition States. Angewandte Chemie - International Edition, 2020, 59, 18686-18694.	7.2	29
29	Hydrogen Chemisorption Isotherms on Platinum Particles at Catalytic Temperatures: Langmuir and Two-Dimensional Gas Models Revisited. Journal of Physical Chemistry C, 2019, 123, 8447-8462.	1.5	28
30	Supraâ€monolayer coverages on small metal clusters and their effects on H₂ chemisorption particle size estimates. AICHE Journal, 2018, 64, 3109-3120.	1.8	24
31	Theoretical insights into the sites and mechanisms for base catalyzed esterification and aldol condensation reactions over Cu. Faraday Discussions, 2017, 197, 59-86.	1.6	23
32	Rigid Arrangements of Ionic Charge in Zeolite Frameworks Conferred by Specific Aluminum Distributions Preferentially Stabilize Alkanol Dehydration Transition States. Angewandte Chemie, 2020, 132, 18845-18853.	1.6	22
33	Oxygen-Doped Carbon Supports Modulate the Hydrogenation Activity of Palladium Nanoparticles through Electronic Metalâ€“Support Interactions. ACS Catalysis, 2022, 12, 7344-7356.	5.5	22
34	Effects of Catalyst Model and High Adsorbate Coverages in ab Initio Studies of Alkane Hydrogenolysis. ACS Catalysis, 2018, 8, 6375-6387.	5.5	21
35	Restructuring of MFI Framework Zeolite Models and Their Associated Artifacts in Density Functional Theory Calculations. Journal of Physical Chemistry C, 2019, 123, 6572-6585.	1.5	21
36	Impact of Metal and Heteroatom Identities in the Hydrogenolysis of Câ€“X Bonds (X = C, N, O, S, and Cl). ACS Catalysis, 2020, 10, 5086-5100.	5.5	21

#	Article	IF	Citations
37	Comparing alkene-mediated and formaldehyde-mediated diene formation routes in methanol-to-olefins catalysis in MFI and CHA. Journal of Catalysis, 2021, 400, 124-139.	3.1	12
38	Mechanism and Effects of Coverage and Particle Morphology on Rh-Catalyzed NOâ€“H₂ Reactions. Journal of Physical Chemistry C, 2020, 124, 13291-13303.	1.5	10
39	Hydrogenation and C S bond activation pathways in thiophene and tetrahydrothiophene reactions on sulfur-passivated surfaces of Ru, Pt, and Re nanoparticles. Applied Catalysis B: Environmental, 2021, 291, 119797.	10.8	9
40	Theoretical and Experimental Characterization of Adsorbed CO and NO on Î³-Al₂O₃-Supported Rh Nanoparticles. Journal of Physical Chemistry C, 2021, 125, 19733-19755.	1.5	9
41	Oxophilicity Drives Oxygen Transfer at a Palladiumâ€“Silver Interface for Increased CO Oxidation Activity. ACS Catalysis, 2020, 10, 13878-13889.	5.5	7
42	Predicting diffusion barriers and diffusivities of C6â€“C12 methylbenzenes in MFI zeolites. Microporous and Mesoporous Materials, 2022, 333, 111705.	2.2	7
43	The Fischer-Tropsch synthesis: A few enduring mechanistic conundrums revisited. Journal of Catalysis, 2022, 405, 614-625.	3.1	7
44	Quantifying Effects of Active Site Proximity on Rates of Methanol Dehydration to Dimethyl Ether over Chabazite Zeolites through Microkinetic Modeling. ACS Materials Au, 2022, 2, 163-175.	2.6	7
45	Binding and Exchange Reactions of Hydrogen Isotopes on Surfaces of Dispersed Pt Nanoparticles. Journal of Physical Chemistry C, 2022, 126, 3923-3938.	1.5	3