Bryan R Goldsmith

List of Publications by Year
in descending order

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44 papers	3,198 citations	304743 22 h-index	289244 40 g-index
45 all docs	45 docs citations	45 times ranked	4301 citing authors

#	Article	IF	Citations
1	Accelerating the structure search of catalysts with machine learning. Current Opinion in Chemical Engineering, 2022, 35, 100771.	7.8	20
2	Explaining the structure sensitivity of Pt and Rh for aqueous-phase hydrogenation of phenol. Journal of Chemical Physics, 2022, 156, 104703.	3.0	7
3	Interpretable machine learning for knowledge generation in heterogeneous catalysis. Nature Catalysis, 2022, 5, 175-184.	34.4	127
4	Recent advances in computational materials design: methods, applications, algorithms, and informatics. Journal of Materials Science, 2022, 57, 10471-10474.	3.7	6
5	Comparing electrocatalytic and thermocatalytic conversion of nitrate on platinumâ€“ruthenium alloys. Catalysis Science and Technology, 2021, 11, 7098-7109.	4.1	18
6	Why halides enhance heterogeneous metal ion charge transfer reactions. Chemical Science, 2021, 12, 12704-12710.	7.4	6
7	The Effect of Anion Bridging on Heterogeneous Charge Transfer for V2+/V3+. Cell Reports Physical Science, 2021, 2, 100307.	5.6	9
8	Increasing electrocatalytic nitrate reduction activity by controlling adsorption through PtRu alloying. Journal of Catalysis, 2021, 395, 143-154.	6.2	94
9	Rhodium Singleâ€Atom Catalysts on Titania for Reverse Water Gas Shift Reaction Explored by First Principles Mechanistic Analysis and Compared to Nanoclusters. ChemCatChem, 2021, 13, 3155-3164.	3.7	10
10	Probing the Influence of Anions on Charge Transfer in Redox Couples for Flow Battery Applications. ECS Meeting Abstracts, 2021, MA2021-01, 212-212.	0.0	0
11	A Proposed Mechanism for the Cerium Electron Transfer for Use in RFB Applications. ECS Meeting Abstracts, 2021, MA2021-01, 211-211.	0.0	0
12	Uncovering electronic and geometric descriptors of chemical activity for metal alloys and oxides using unsupervised machine learning. Chem Catalysis, 2021, 1, 923-940.	6.1	22
13	Perovskite oxynitrides as tunable materials for electrocatalytic nitrogen reduction to ammonia. Trends in Chemistry, 2021, 3, 694-696.	8.5	6
14	Electrocatalytic nitrate reduction on rhodium sulfide compared to Pt and Rh in the presence of chloride. Catalysis Science and Technology, 2021, 11, 7331-7346.	4.1	13
15	(Invited) Probing the Reaction Mechanism of the Electrocatalytic Reduction of Nitrate. ECS Meeting Abstracts, 2021, MA2021-02, 1553-1553.	0.0	0
16	Theory-Guided Machine Learning Finds Geometric Structure-Property Relationships for Chemisorption on Subsurface Alloys. CheM, 2020, 6, 3100-3117.	11.7	65
17	Nanocluster and single-atom catalysts for thermocatalytic conversion of CO and CO₂. Catalysis Science and Technology, 2020, 10, 5772-5791.	4.1	32
18	Structures and Free Energies of Cerium Ions in Acidic Electrolytes. Inorganic Chemistry, 2020, 59, 12552-12563.	4.0	14

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19	Inorganic Halide Double Perovskites with Optoelectronic Properties Modulated by Sublattice Mixing. Journal of the American Chemical Society, 2020, 142, 5135-5145.	13.7	62
20	Role of Electrocatalysis in the Remediation of Water Pollutants. ACS Catalysis, 2020, 10, 3365-3371.	11.2	88
21	Adsorption Energies of Oxygenated Aromatics and Organics on Rhodium and Platinum in Aqueous Phase. ACS Catalysis, 2020, 10, 4929-4941.	11.2	37
22	Structures and Free Energies of Cerium Ions in Acidic Electrolytes and Structures of Electrolyte-Electrode Interfaces to Inform Kinetic Performance in Redox Flow Battery Applications. ECS Meeting Abstracts, 2020, MA2020-02, 714-714.	0.0	0
23	Increasing Electrocatalytic Nitrate Reduction Performance By Tuning Adsorption through PtRu Alloying. ECS Meeting Abstracts, 2020, MA2020-02, 3267-3267.	0.0	1
24	Surpassing the single-atom catalytic activity limit through paired Pt-O-Pt ensemble built from isolated Pt1 atoms. Nature Communications, 2019, 10, 3808.	12.8	225
25	Nitrogen-doped graphene layers for electrochemical oxygen reduction reaction boosted by lattice strain. Journal of Catalysis, 2019, 378, 113-120.	6.2	19
26	V²⁺/V³⁺ Redox Kinetics on Glassy Carbon in Acidic Electrolytes for Vanadium Redox Flow Batteries. ACS Energy Letters, 2019, 4, 2368-2377.	17.4	36
27	Activity and Selectivity Trends in Electrocatalytic Nitrate Reduction on Transition Metals. ACS Catalysis, 2019, 9, 7052-7064.	11.2	369
28	New tolerance factor to predict the stability of perovskite oxides and halides. Science Advances, 2019, 5, eaav0693.	10.3	778
29	Two-to-three dimensional transition in neutral gold clusters: The crucial role of van der Waals interactions and temperature. Physical Review Materials, 2019, 3, .	2.4	40
30	Machine learning for heterogeneous catalyst design and discovery. AICHE Journal, 2018, 64, 2311-2323.	3.6	258
31	Uncovering structure-property relationships of materials by subgroup discovery. New Journal of Physics, 2017, 19, 013031.	2.9	77
32	Beyond Ordered Materials: Understanding Catalytic Sites on Amorphous Solids. ACS Catalysis, 2017, 7, 7543-7557.	11.2	134
33	Identifying consistent statements about numerical data with dispersion-corrected subgroup discovery. Data Mining and Knowledge Discovery, 2017, 31, 1391-1418.	3.7	23
34	Synthesis and Characterization of a Cu₁₄ Hydride Cluster Supported by Neutral Donor Ligands. Chemistry - A European Journal, 2015, 21, 5341-5344.	3.3	60
35	Rate-Enhancing Roles of Water Molecules in Methyltrioxorhenium-Catalyzed Olefin Epoxidation by Hydrogen Peroxide. Journal of the American Chemical Society, 2015, 137, 9604-9616.	13.7	42
36	A Cu₂₅ Nanocluster with Partial Cu(0) Character. Journal of the American Chemical Society, 2015, 137, 13319-13324.	13.7	234

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37	CO- and NO-Induced Disintegration and Redispersion of Three-Way Catalysts Rhodium, Palladium, and Platinum: An ab Initio Thermodynamics Study. Journal of Physical Chemistry C, 2014, 118, 9588-9597.	3.1	56
38	Isolated catalyst sites on amorphous supports: A systematic algorithm for understanding heterogeneities in structure and reactivity. Journal of Chemical Physics, 2013, 138, 204105.	3.0	41
39	Water-Catalyzed Activation of H₂O₂ by Methyltrioxorhenium: A Combined Computationalâ€“Experimental Study. Inorganic Chemistry, 2013, 52, 13904-13917.	4.0	20
40	Synthesis and Micropatterning of Photocatalytically Reactive Self-Assembled Monolayers Covalently Linked to Si(100) Surfaces via a Siâ€“C Bond. Langmuir, 2012, 28, 16156-16166.	3.5	7
41	Solventâ€Free Conversion of Linalool to Methylcyclopentadiene Dimers: A Route To Renewable Highâ€Density Fuels. ChemSusChem, 2011, 4, 465-469.	6.8	110
42	Template Assisted Growth and Characterization of Electrodeposited Permalloy(Ni₈₀Fe₂₀)/Cu Multilayered Nanowires. ECS Transactions, 2010, 25, 97-103.	0.5	2
43	Synthesis and characterization of electrodeposited permalloy (Ni80Fe20)/Cu multilayered nanowires. Journal of Magnetism and Magnetic Materials, 2010, 322, 3876-3881.	2.3	25
44	CHAPTER 9. Understanding Reactivity with Reduced Potential Energy Landscapes: Recent Advances and New Directions. RSC Theoretical and Computational Chemistry Series, 0, , 213-232.	0.7	4