Geun Ho Gu

List of Publications by Year
in descending order

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25	1,241	471509 17	552781 26
papers	citations	h-index	g-index

26	26	26	1578
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Machine learning for renewable energy materials. Journal of Materials Chemistry A, 2019, 7, 17096-17117.	10.3	207
2	Guaiacol Hydrodeoxygenation Mechanism on Pt(111): Insights from Density Functional Theory and Linear Free Energy Relations. ChemSusChem, 2015, 8, 315-322.	6.8	109
3	Highly stable two-dimensional bismuth metal-organic frameworks for efficient electrochemical reduction of CO2. Applied Catalysis B: Environmental, 2020, 277, 119241.	20.2	109
4	Generative Adversarial Networks for Crystal Structure Prediction. ACS Central Science, 2020, 6, 1412-1420.	11.3	102
5	Machine-enabled inverse design of inorganic solid materials: promises and challenges. Chemical Science, 2020, 11, 4871-4881.	7.4	88
6	Understanding potential-dependent competition between electrocatalytic dinitrogen and proton reduction reactions. Nature Communications, 2021, 12, 4353.	12.8	78
7	Mechanism of Dehydration of Phenols on Noble Metals via First-Principles Microkinetic Modeling. ACS Catalysis, 2016, 6, 3047-3055.	11.2	69
8	Reduced graphene oxides with engineered defects enable efficient electrochemical reduction of dinitrogen to ammonia in wide pH range. Nano Energy, 2020, 68, 104323.	16.0	64
9	Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening. Journal of Physical Chemistry Letters, 2020, 11, 3185-3191.	4.6	63
10	Structure-Based Synthesizability Prediction of Crystals Using Partially Supervised Learning. Journal of the American Chemical Society, 2020, 142, 18836-18843.	13.7	59
11	Progress in Computational and Machineâ€Learning Methods for Heterogeneous Smallâ€Molecule Activation. Advanced Materials, 2020, 32, e1907865.	21.0	46
12	Autobifunctional Mechanism of Jagged Pt Nanowires for Hydrogen Evolution Kinetics via End-to-End Simulation. Journal of the American Chemical Society, 2021, 143, 5355-5363.	13.7	33
13	Uncertainty-Quantified Hybrid Machine Learning/Density Functional Theory High Throughput Screening Method for Crystals. Journal of Chemical Information and Modeling, 2020, 60, 1996-2003.	5.4	31
14	Thermochemistry of gas-phase and surface speciesviaLASSO-assisted subgraph selection. Reaction Chemistry and Engineering, 2018, 3, 454-466.	3.7	29
15	Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111). Journal of Physical Chemistry C, 2017, 121, 21510-21519.	3.1	27
16	Lattice Convolutional Neural Network Modeling of Adsorbate Coverage Effects. Journal of Physical Chemistry C, 2019, 123, 18951-18959.	3.1	21
17	Group Additivity for Thermochemical Property Estimation of Lignin Monomers on Pt(111). Journal of Physical Chemistry C, 2016, 120, 19234-19241.	3.1	18
18	Unveiling new stable manganese based photoanode materials via theoretical high-throughput screening and experiments. Chemical Communications, 2019, 55, 13418-13421.	4.1	18

#	Article	IF	Citations
19	Perovskite synthesizability using graph neural networks. Npj Computational Materials, 2022, 8, .	8.7	16
20	Bimetallic Goldâ€“Silver Nanostructures Drive Low Overpotentials for Electrochemical Carbon Dioxide Reduction. ACS Applied Materials & Interfaces, 2022, 14, 6604-6614.	8.0	14
21	Microkinetic modeling of aqueous phase biomass conversion: Application to ethylene glycol reforming. Chemical Engineering Science, 2019, 197, 415-418.	3.8	12
22	Uncertainty Quantification and Error Propagation in the Enthalpy and Entropy of Surface Reactions Arising from a Single DFT Functional. Journal of Physical Chemistry C, 2021, 125, 18187-18196.	3.1	8
23	Automated exploitation of the big configuration space of large adsorbates on transition metals reveals chemistry feasibility. Nature Communications, 2022, 13, 2087.	12.8	8
24	Tailoring electrode hydrophobicity to improve anode performance in alkaline media. Journal of Power Sources, 2013, 242, 581-588.	7.8	7
25	Predicting potentially hazardous chemical reactions using an explainable neural network. Chemical Science, 2021, 12, 11028-11037.	7.4	3