Egill Skulason

List of Publications by Year
in descending order

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Version: 2024-02-01

55	8,695	136885	138417
papers	citations	32 h-index	58 g-index

58	58	58	8387
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Scaling Properties of Adsorption Energies for Hydrogen-Containing Molecules on Transition-Metal Surfaces. Physical Review Letters, 2007, 99, 016105.	2.9	1,270
2	A theoretical evaluation of possible transition metal electro-catalysts for N₂reduction. Physical Chemistry Chemical Physics, 2012, 14, 1235-1245.	1.3	1,184
3	Modeling the Electrochemical Hydrogen Oxidation and Evolution Reactions on the Basis of Density Functional Theory Calculations. Journal of Physical Chemistry C, 2010, 114, 18182-18197.	1.5	990
4	Density functional theory calculations for the hydrogen evolution reaction in an electrochemical double layer on the Pt(111) electrode. Physical Chemistry Chemical Physics, 2007, 9, 3241-3250.	1.3	678
5	The oxygen reduction reaction mechanism on Pt(111) from density functional theory calculations. Electrochimica Acta, 2010, 55, 7975-7981.	2.6	491
6	Universal transition state scaling relations for (de)hydrogenation over transition metals. Physical Chemistry Chemical Physics, 2011, 13, 20760.	1.3	363
7	Modeling the electrified solidâ€“liquid interface. Chemical Physics Letters, 2008, 466, 68-71.	1.2	349
8	Electroreduction of N₂ to Ammonia at Ambient Conditions on Mononitrides of Zr, Nb, Cr, and V: A DFT Guide for Experiments. ACS Catalysis, 2016, 6, 635-646.	5.5	317
9	Enabling electrochemical reduction of nitrogen to ammonia at ambient conditions through rational catalyst design. Physical Chemistry Chemical Physics, 2015, 17, 4909-4918.	1.3	246
10	Calculations of Product Selectivity in Electrochemical CO₂ Reduction. ACS Catalysis, 2018, 8, 5240-5249.	5.5	203
11	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192
12	Cyclic Voltammograms for H on Pt(111) and Pt(100) from First Principles. Physical Review Letters, 2007, 99, 126101.	2.9	189
13	Onset potentials for different reaction mechanisms of nitrogen activation to ammonia on transition metal nitride electro-catalysts. Catalysis Today, 2017, 286, 69-77.	2.2	164
14	Hydrogen adsorption on palladium and palladium hydride at 1 bar. Surface Science, 2010, 604, 718-729.	0.8	158
15	Hydrogenation of CO₂ to Methanol by Pt Nanoparticles Encapsulated in UiO-67: Deciphering the Role of the Metalâ€“Organic Framework. Journal of the American Chemical Society, 2020, 142, 999-1009.	6.6	141
16	Standard hydrogen electrode and potential of zero charge in density functional calculations. Physical Review B, 2011, 84, .	1.1	118
17	Electrochemical synthesis of ammonia via Mars-van Krevelen mechanism on the (111) facets of group IIIâ€“VII transition metal mononitrides. Catalysis Today, 2017, 286, 78-84.	2.2	117
18	Computational Screening of Rutile Oxides for Electrochemical Ammonia Formation. ACS Sustainable Chemistry and Engineering, 2017, 5, 10327-10333.	3.2	115

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19	Hydrogen Evolution Reaction Catalyzed by Transition-Metal Nitrides. Journal of Physical Chemistry C, 2017, 121, 24036-24045.	1.5	108
20	A systematic DFT study of hydrogen diffusion on transition metal surfaces. Surface Science, 2012, 606, 1400-1404.	0.8	104
21	Computational Predictions of Catalytic Activity of Zincblende (110) Surfaces of Metal Nitrides for Electrochemical Ammonia Synthesis. Journal of Physical Chemistry C, 2017, 121, 6141-6151.	1.5	99
22	On the pH dependence of electrochemical proton transfer barriers. Catalysis Today, 2016, 262, 36-40.	2.2	91
23	Elucidating the Mechanism of Electrochemical N₂ Reduction at the Ru(0001) Electrode. ACS Catalysis, 2019, 9, 11137-11145.	5.5	78
24	Assessment of Constant-Potential Implicit Solvation Calculations of Electrochemical Energy Barriers for H₂ Evolution on Pt. Journal of Physical Chemistry C, 2019, 123, 4116-4124.	1.5	71
25	Influence of Defects and H₂O on the Hydrogenation of CO₂ to Methanol over Pt Nanoparticles in UiO-67 Metalâ€“Organic Framework. Journal of the American Chemical Society, 2020, 142, 17105-17118.	6.6	68
26	Hydrogen adsorption and desorption at the Pt(110)-(1Ã—2) surface: experimental and theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 6323.	1.3	67
27	The Mechanism of Industrial Ammonia Synthesis Revisited: Calculations of the Role of the Associative Mechanism. Journal of Physical Chemistry C, 2015, 119, 26554-26559.	1.5	60
28	Trends of Electrochemical CO₂ Reduction Reaction on Transition Metal Oxide Catalysts. Journal of Physical Chemistry C, 2018, 122, 10078-10087.	1.5	54
29	Faraday efficiency and mechanism of electrochemical surface reactions: CO₂ reduction and H₂ formation on Pt(111). Faraday Discussions, 2016, 195, 619-636.	1.6	45
30	Local density of states analysis using Bader decomposition for N2 and CO2 adsorbed on Pt(110)-(1â€‰Ã—â€‰2) electrodes. Journal of Chemical Physics, 2012, 137, 164705.	1.2	39
31	Are There Any Overlooked Catalysts for Electrochemical NH3 Synthesisâ€”New Insights from Analysis of Thermochemical Data. IScience, 2020, 23, 101803.	1.9	36
32	Biomimetic Nitrogen Fixation Catalyzed by Transition Metal Sulfide Surfaces in an Electrolytic Cell. ChemSusChem, 2019, 12, 4265-4273.	3.6	35
33	Preparation of Nafion Membranes for Reproducible Ammonia Quantification in Nitrogen Reduction Reaction Experiments. Angewandte Chemie - International Edition, 2020, 59, 22938-22942.	7.2	31
34	A density functional theory study of the mechanism and onset potentials for the major products of NO electroreduction on transition metal catalysts. Applied Surface Science, 2021, 552, 149063.	3.1	28
35	Catalytic trends of nitrogen doped carbon nanotubes for oxygen reduction reaction. Nanoscale, 2019, 11, 18683-18690.	2.8	27
36	Catalytic Activity of Pt Nano-Particles for H2 Formation. Topics in Catalysis, 2014, 57, 273-281.	1.3	26

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37	Computational Study of Electrochemical CO2 Reduction at Transition Metal Electrodes. Procedia Computer Science, 2015, 51, 1865-1871.	1.2	26
38	C₃ production from CO₂ reduction by concerted *CO trimerization on a single-atom alloy catalyst. Journal of Materials Chemistry A, 2022, 10, 5998-6006.	5.2	25
39	Reentrant Mechanism for Associative Desorption:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:mi>Pt</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo stretchy="false">)</mml:mo><mml:mtext mathvariant="normal">â^’</mml:mtext><mml:mo		

#	Article	IF	Citations
55	Cyclic Voltammograms from First Principles. ECS Transactions, 2007, 11, 759-768.	0.3	2