Egill Skulason

List of Publications by Year
in descending order

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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	Optimizing Nitrogen Reduction Reaction on Nitrides: A Computational Study on Crystallographic Orientation. Topics in Catalysis, 2022, 65, 252-261.	1.3	14
2	Investigation into the mechanism of electrochemical nitrogen reduction reaction to ammonia using niobium oxynitride thin-film catalysts. Electrochimica Acta, 2022, 403, 139551.	2.6	19
3	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
4	Perspectives on the Competition between the Electrochemical Water and N₂ Oxidation on a TiO₂(110) Electrode. Journal of Physical Chemistry Letters, 2022, 13, 6123-6129.	2.1	10
5	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
6	Assessment of the Accuracy of Density Functionals for Calculating Oxygen Reduction Reaction on Nitrogen-Doped Graphene. Journal of Chemical Theory and Computation, 2021, 17, 6405-6415.	2.3	9
7	Effect of co-adsorbed water on electrochemical CO2 reduction reaction on transition metal oxide catalysts. Applied Surface Science, 2021, 570, 151031.	3.1	7
8	Computational examination of the kinetics of electrochemical nitrogen reduction and hydrogen evolution on a tungsten electrode. Journal of Catalysis, 2021, 404, 362-370.	3.1	12
9	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
10	Why do RuO₂ electrodes catalyze electrochemical CO₂ reduction to methanol rather than methane or perhaps neither of those?. Chemical Science, 2020, 11, 9542-9553.	3.7	17
11	Preparation of Nafion Membranes for Reproducible Ammonia Quantification in Nitrogen Reduction Reaction Experiments. Angewandte Chemie - International Edition, 2020, 59, 22938-22942.	7.2	31
12	Preparation of Nafion Membranes for Reproducible Ammonia Quantification in Nitrogen Reduction Reaction Experiments. Angewandte Chemie, 2020, 132, 23138-23142.	1.6	16
13	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
14	Are There Any Overlooked Catalysts for Electrochemical NH3 Synthesisâ€”New Insights from Analysis of Thermochemical Data. IScience, 2020, 23, 101803.	1.9	36
15	Mechanisms and Potential-Dependent Energy Barriers for Hydrogen Evolution on Supported MoS₂ Catalysts. Journal of Physical Chemistry C, 2020, 124, 17015-17026.	1.5	9
16	Elucidation of temperature-programmed desorption of high-coverage hydrogen on Pt(211), Pt(221), Pt(533) and Pt(553) based on density functional theory calculations. Physical Chemistry Chemical Physics, 2019, 21, 17142-17151.	1.3	10
17	Biomimetic Nitrogen Fixation Catalyzed by Transition Metal Sulfide Surfaces in an Electrolytic Cell. ChemSusChem, 2019, 12, 4265-4273.	3.6	35
18	Elucidating the Mechanism of Electrochemical N₂ Reduction at the Ru(0001) Electrode. ACS Catalysis, 2019, 9, 11137-11145.	5.5	78

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19	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
20	Catalytic trends of nitrogen doped carbon nanotubes for oxygen reduction reaction. Nanoscale, 2019, 11, 18683-18690.	2.8	27
21	Geometric and Electronic Effects Contributing to N₂ Dissociation Barriers on a Range of Active Sites on Ru Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 30458-30466.	1.5	13
22	Calculations of Product Selectivity in Electrochemical CO₂ Reduction. ACS Catalysis, 2018, 8, 5240-5249.	5.5	203
23	Trends of Electrochemical CO₂ Reduction Reaction on Transition Metal Oxide Catalysts. Journal of Physical Chemistry C, 2018, 122, 10078-10087.	1.5	54
24	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
25	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
26	Atomic scale simulations of heterogeneous electrocatalysis: recent advances. Advances in Physics: X, 2017, 2, 481-495.	1.5	18
27	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
28	Hydrogen Evolution Reaction Catalyzed by Transition-Metal Nitrides. Journal of Physical Chemistry C, 2017, 121, 24036-24045.	1.5	108
29	Computational Screening of Rutile Oxides for Electrochemical Ammonia Formation. ACS Sustainable Chemistry and Engineering, 2017, 5, 10327-10333.	3.2	115
30	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
31	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
32	On the pH dependence of electrochemical proton transfer barriers. Catalysis Today, 2016, 262, 36-40.	2.2	91
33	Computational Study of Electrochemical CO2 Reduction at Transition Metal Electrodes. Procedia Computer Science, 2015, 51, 1865-1871.	1.2	26
34	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
35	Modeling Electrochemical Reactions at the Solid-liquid Interface Using Density Functional Calculations. Procedia Computer Science, 2015, 51, 1887-1896.	1.2	15
36	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

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37	A systematic, first-principles study of the structural preference and magnetic properties of mononitrides of the d-block metals. Journal of Alloys and Compounds, 2014, 603, 172-179.	2.8	22
38	Catalytic Activity of Pt Nano-Particles for H2 Formation. Topics in Catalysis, 2014, 57, 273-281.	1.3	26
39	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
40	Modeling of the symmetry factor of electrochemical proton discharge via the Volmer reaction. Catalysis Today, 2013, 202, 168-174.	2.2	16
41	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
42	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		

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55	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192