Heine A Hansen

List of Publications by Year
in descending order

101	15,582	50170 46	43802 91
papers	citations	h-index	g-index

105	105	105	16231
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. ChemCatChem, 2011, 3, 1159-1165.	1.8	3,208
2	Alloys of platinum and early transition metals as oxygen reduction electrocatalysts. Nature Chemistry, 2009, 1, 552-556.	6.6	2,716
3	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	0.7	1,451
4	Understanding Trends in the Electrocatalytic Activity of Metals and Enzymes for CO₂ Reduction to CO. Journal of Physical Chemistry Letters, 2013, 4, 388-392.	2.1	604
5	Surface Pourbaix diagrams and oxygen reduction activity of Pt, Ag and Ni(111) surfaces studied by DFT. Physical Chemistry Chemical Physics, 2008, 10, 3722.	1.3	480
6	Universality in Oxygen Reduction Electrocatalysis on Metal Surfaces. ACS Catalysis, 2012, 2, 1654-1660.	5.5	456
7	Trends in electrochemical CO2 reduction activity for open and close-packed metal surfaces. Physical Chemistry Chemical Physics, 2014, 16, 4720.	1.3	375
8	Unifying Kinetic and Thermodynamic Analysis of 2 e^{â€“} and 4 e^{â€“} Reduction of Oxygen on Metal Surfaces. Journal of Physical Chemistry C, 2014, 118, 6706-6718.	1.5	337
9	Direct observation of the oxygenated species during oxygen reduction on a platinum fuel cell cathode. Nature Communications, 2013, 4, .	5.8	325
10	Electrochemical chlorine evolution at rutile oxide (110) surfaces. Physical Chemistry Chemical Physics, 2010, 12, 283-290.	1.3	317
11	Scaling Relationships for Adsorption Energies on Transition Metal Oxide, Sulfide, and Nitride Surfaces. Angewandte Chemie - International Edition, 2008, 47, 4683-4686.	7.2	301
12	Towards identifying the active sites on RuO₂(110) in catalyzing oxygen evolution. Energy and Environmental Science, 2017, 10, 2626-2637.	15.6	278
13	Unifying the 2e^{â€“} and 4e^{â€“} Reduction of Oxygen on Metal Surfaces. Journal of Physical Chemistry Letters, 2012, 3, 2948-2951.	2.1	276
14	Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO₂ Reduction. ChemCatChem, 2014, 6, 1899-1905.	1.8	255
15	Orientation-Dependent Oxygen Evolution on RuO₂ without Lattice Exchange. ACS Energy Letters, 2017, 2, 876-881.	8.8	251
16	Method for locating low-energy solutions within<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>DFT</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>. Physical Review B, 2010, 82, .	1.1	215
17	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. Physical Chemistry Chemical Physics, 2012, 14, 49-70.	1.3	198
18	The Pt(111)/Electrolyte Interface under Oxygen Reduction Reaction Conditions: An Electrochemical Impedance Spectroscopy Study. Langmuir, 2011, 27, 2058-2066.	1.6	170

#	Article	IF	Citations
19	Identifying systematic DFT errors in catalytic reactions. Catalysis Science and Technology, 2015, 5, 4946-4949.	2.1	144
20	Selective Electrochemical Generation of Hydrogen Peroxide from Water Oxidation. Journal of Physical Chemistry Letters, 2015, 6, 4224-4228.	2.1	142
21	Bifunctional alloys for the electroreduction of CO₂and CO. Physical Chemistry Chemical Physics, 2016, 18, 9194-9201.	1.3	127
22	Mechanistic Pathway in the Electrochemical Reduction of CO2 on RuO2. ACS Catalysis, 2015, 5, 4075-4081.	5.5	123
23	Functional Independent Scaling Relation for ORR/OER Catalysts. Journal of Physical Chemistry C, 2016, 120, 24910-24916.	1.5	119
24	Synthesis of thin film AuPd alloys and their investigation for electrocatalytic CO₂reduction. Journal of Materials Chemistry A, 2015, 3, 20185-20194.	5.2	116
25	Opportunities and challenges in the electrocatalysis of CO2 and CO reduction using bifunctional surfaces: A theoretical and experimental study of Auâ€“Cd alloys. Journal of Catalysis, 2016, 343, 215-231.	3.1	115
26	2D transition metalâ€“TCNQ sheets as bifunctional single-atom catalysts for oxygen reduction and evolution reaction (ORR/OER). Journal of Catalysis, 2019, 370, 378-384.	3.1	114
27	Electrochemical reduction of CO2 on compositionally variant Au-Pt bimetallic thin films. Nano Energy, 2017, 42, 51-57.	8.2	99
28	Elucidating the activity of stepped Pt single crystals for oxygen reduction. Physical Chemistry Chemical Physics, 2014, 16, 13625.	1.3	92
29	Kinetics and Thermodynamics of H₂O Dissociation on Reduced CeO₂(111). Journal of Physical Chemistry C, 2014, 118, 27402-27414.	1.5	91
30	Formation energies of rutile metal dioxides using density functional theory. Physical Review B, 2009, 79, .	1.1	87
31	DFT study of stabilization effects on N-doped graphene for ORR catalysis. Catalysis Today, 2018, 312, 118-125.	2.2	81
32	Modeling CO2 reduction on Pt(111). Physical Chemistry Chemical Physics, 2013, 15, 7114.	1.3	80
33	Cation insertion to break the activity/stability relationship for highly active oxygen evolution reaction catalyst. Nature Communications, 2020, 11, 1378.	5.8	79
34	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101.	1.2	77
35	OH formation and H₂ adsorption at the liquid waterâ€“Pt(111) interface. Chemical Science, 2018, 9, 6912-6921.	3.7	76
36	Simulating Linear Sweep Voltammetry from First-Principles: Application to Electrochemical Oxidation of Water on Pt(111) and Pt₃Ni(111). Journal of Physical Chemistry C, 2012, 116, 4698-4704.	1.5	71

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37	Niâ€“Feâ€“S Cubanes in CO₂ Reduction Electrocatalysis: A DFT Study. ACS Catalysis, 2013, 3, 2640-2643.	5.5	68
38	Ternary ruthenium complex hydrides for ammonia synthesis via the associative mechanism. Nature Catalysis, 2021, 4, 959-967.	16.1	67
39	A DFT-based genetic algorithm search for AuCu nanoalloy electrocatalysts for CO₂ reduction. Physical Chemistry Chemical Physics, 2015, 17, 28270-28276.	1.3	65
40	Acid-Stable and Active Mâ€“Nâ€“C Catalysts for the Oxygen Reduction Reaction: The Role of Local Structure. ACS Catalysis, 2021, 11, 13102-13118.	5.5	59
41	Enhanced Oxygen Reduction Activity by Selective Anion Adsorption on Non-Precious-Metal Catalysts. ACS Catalysis, 2018, 8, 7104-7112.	5.5	53
42	Giant onsite electronic entropy enhances the performance of ceria for water splitting. Nature Communications, 2017, 8, 285.	5.8	51
43	From 3D to 2D Co and Ni Oxyhydroxide Catalysts: Elucidation of the Active Site and Influence of Doping on the Oxygen Evolution Activity. ACS Catalysis, 2017, 7, 8558-8571.	5.5	50
44	Volcano Relation for the Deacon Process over Transitionâ€Metal Oxides. ChemCatChem, 2010, 2, 98-102.	1.8	49
45	Pt Skin Versus Pt Skeleton Structures of Pt3Sc as Electrocatalysts for Oxygen Reduction. Topics in Catalysis, 2014, 57, 245-254.	1.3	47
46	Comparative DFT+U and HSE Study of the Oxygen Evolution Electrocatalysis on Perovskite Oxides. Journal of Physical Chemistry C, 2018, 122, 1135-1147.	1.5	46
47	DFT Study of the Oxygen Reduction Reaction on Carbon-Coated Iron and Iron Carbide. ACS Catalysis, 2018, 8, 10521-10529.	5.5	46
48	First principles investigation of zinc-anode dissolution in zincâ€“air batteries. Physical Chemistry Chemical Physics, 2013, 15, 6416.	1.3	44
49	Ti atoms in Ru0.3Ti0.7O2 mixed oxides form active and selective sites for electrochemical chlorine evolution. Electrochimica Acta, 2014, 146, 733-740.	2.6	44
50	First principles investigation of the activity of thin film Pt, Pd and Au surface alloys for oxygen reduction. Physical Chemistry Chemical Physics, 2015, 17, 11647-11657.	1.3	41
51	Computational Screening of Doped Î±â€MnO₂ Catalysts for the Oxygen Evolution Reaction. ChemSusChem, 2018, 11, 629-637.	3.6	40
52	Universality in Nonaqueous Alkali Oxygen Reduction on Metal Surfaces: Implications for Liâ€“O₂ and Naâ€“O₂ Batteries. ACS Energy Letters, 2016, 1, 162-168.	8.8	39
53	Improved Electrocatalytic Water Splitting Reaction on CeO₂(111) by Strain Engineering: A DFT+U Study. ACS Catalysis, 2019, 9, 4853-4861.	5.5	37
54	Nanoscale structural characterization of Mg(NH3)6Cl2 during NH3 desorption: An in situ small angle X-ray scattering study. Chemical Physics Letters, 2007, 441, 255-260.	1.2	35

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55	Unifying Solution and Surface Electrochemistry: Limitations and Opportunities in Surface Electrocatalysis. Topics in Catalysis, 2014, 57, 215-221.	1.3	35
56	Descriptors and Thermodynamic Limitations of Electrocatalytic Carbon Dioxide Reduction on Rutile Oxide Surfaces. ChemSusChem, 2016, 9, 3230-3243.	3.6	34
57	Improving the Activity of Mâ^'N₄ Catalysts for the Oxygen Reduction Reaction by Electrolyte Adsorption. ChemSusChem, 2019, 12, 5133-5141.	3.6	33
58	Facet-dependent electrocatalytic water splitting reaction on CeO2: A DFTÂ+ÂU study. Journal of Catalysis, 2020, 388, 1-10.	3.1	32
59	Mechanism of Water Splitting on Gadolinium-Doped CeO₂(111): A DFT + U Study. Journal of Physical Chemistry C, 2019, 123, 5507-5517.	1.5	31
60	Reducing Systematic Errors in Oxide Species with Density Functional Theory Calculations. Journal of Physical Chemistry C, 2015, 119, 17596-17601.	1.5	29
61	Vanadium oxynitrides as stable catalysts for electrochemical reduction of nitrogen to ammonia: the role of oxygen. Journal of Materials Chemistry A, 2020, 8, 24098-24107.	5.2	29
62	Decoupling strain and ligand effects in ternary nanoparticles for improved ORR electrocatalysis. Physical Chemistry Chemical Physics, 2016, 18, 24737-24745.	1.3	26
63	A comparison of single and double Co sites incorporated in N-doped graphene for the oxygen reduction reaction. Journal of Catalysis, 2021, 393, 230-237.	3.1	26
64	Using microkinetic analysis to search for novel anhydrous formaldehyde production catalysts. Surface Science, 2015, 641, 105-111.	0.8	25
65	Energyâ€“entropy competition in cationâ€“hydroxyl interactions at the liquid waterâ€“Pt(111) interface. Chemical Communications, 2020, 56, 427-430.	2.2	25
66	Combined DFT and Differential Electrochemical Mass Spectrometry Investigation of the Effect of Dopants in Secondary Zincâ€“Air Batteries. ChemSusChem, 2018, 11, 1933-1941.	3.6	23
67	Electroreduction of Methanediol on Copper. Catalysis Letters, 2013, 143, 631-635.	1.4	21
68	Combinatorial selection of a two-dimensional 3d-TM-tetracyanoquinodimethane (TM-TCNQ) monolayer as a high-activity nanocatalyst for CO oxidation. Physical Chemistry Chemical Physics, 2018, 20, 5173-5179.	1.3	21
69	Nâ€Ðoped Graphene Supported on Metalâ€Iron Carbide as a Catalyst for the Oxygen Reduction Reaction: Density Functional Theory Study. ChemSusChem, 2020, 13, 996-1005.	3.6	21
70	Pyridinic-Type N-Doped Graphene on Cobalt Substrate as Efficient Electrocatalyst for Oxygen Reduction Reaction in Acidic Solution in Fuel Cell. Journal of Physical Chemistry Letters, 2021, 12, 3552-3559.	2.1	20
71	1D metal-dithiolene wires as a new class of bi-functional oxygen reduction and evolution single-atom electrocatalysts. Journal of Catalysis, 2021, 393, 140-148.	3.1	18
72	Electrochemical Reduction of CO2 on IrxRu(1â€“x)O2(110) Surfaces. ACS Catalysis, 2017, 7, 8502-8513.	5.5	16

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73	The Role of Oxygenic Groups and sp³ Carbon Hybridization in Activated Graphite Electrodes for Vanadium Redox Flow Batteries. ChemSusChem, 2021, 14, 3945-3952.	3.6	16
74	Formation of a Complex Active Center by Ba₂RuH₆ for Nondissociative Dinitrogen Activation and Ammonia Formation. ACS Catalysis, 2022, 12, 4194-4202.	5.5	15
75	Role of CO* as a Spectator in CO2 Electroreduction on RuO2. Journal of Physical Chemistry C, 2017, 121, 18333-18343.	1.5	14
76	DFT + U Study of Strain-Engineered CO2 Reduction on a CeO2â€“x (111) Facet. Journal of Physical Chemistry C, 2021, 125, 14221-14227.	1.5	14
77	Rate enhancement in microfabricated chemical reactors under fast forced temperature oscillations. Catalysis Communications, 2006, 7, 272-275.	1.6	13
78	CO2 activation at Au(110)â€“water interfaces: An ab initio molecular dynamics study. Journal of Chemical Physics, 2021, 155, 134703.	1.2	13
79	Computational Study of Nb-Doped-SnO₂/Pt Interfaces: Dopant Segregation, Electronic Transport, and Catalytic Properties. Chemistry of Materials, 2017, 29, 1641-1649.	3.2	12
80	Volcano Relations for Oxidation of Hydrogen Halides over Rutile Oxide Surfaces. ChemCatChem, 2012, 4, 1856-1861.	1.8	11
81	The role of nitrogen and sulfur dual coordination of cobalt in Co-N_{4â^'x}S_x/C single atom catalysts in the oxygen reduction reaction. Sustainable Energy and Fuels, 2021, 6, 179-187.	2.5	10
82	Unfolding the structural stability of nanoalloys via symmetry-constrained genetic algorithm and neural network potential. Npj Computational Materials, 2022, 8, .	3.5	9
83	DFT+U study of CO2 reduction and CO oxidation on a reconstructed CeO2â^'(110) facet. Materials Today Advances, 2020, 8, 100111.	2.5	8
84	Structure and energetics of liquid waterâ€“hydroxyl layers on Pt(111). Physical Chemistry Chemical Physics, 2022, 24, 9885-9890.	1.3	8
85	Enhanced activity for electrocatalytic H2 production through cooperative Pr and Bi co-doping of CeO2 in solid oxide electrolysis cells. Journal of Catalysis, 2021, 402, 310-314.	3.1	7
86	Metalâ€Doped PdH(111) Catalysts for CO₂ Reduction. ChemSusChem, 2022, 15, .	3.6	7
87	Layered double hydroxides as advanced tracks to promote ionic conductivity in metal borohydride. Materials Chemistry Frontiers, 2021, 5, 4989-4996.	3.2	6
88	Degradation of polybenzimidazole in alkaline solution with first-principles Modeling. Electrochimica Acta, 2021, 398, 139329.	2.6	5
89	Role of macrocyclic salen-type Schiff base ligands in one-dimensional Co(II) complexes for superior activities toward oxygen reduction/evolution reactions. International Journal of Hydrogen Energy, 2022, 47, 27000-27011.	3.8	5
90	DFT Studies of the Oxygen Reduction Reaction on Pristine and N-Doped Fe3C/Graphene Catalyst. ECS Meeting Abstracts, 2016, , .	0.0	0

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91	Tailoring the Performance of Oxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2016, , .	0.0	0
92	ORR Activity of Pristine Graphite | Fe3c Interfaces. ECS Meeting Abstracts, 2016, , .	0.0	0
93	(Invited) Genetic Algorithms and DFT for Accelerated Design of Nanoalloys. ECS Meeting Abstracts, 2016, , .	0.0	0
94	Understanding and Tailoring the Performance of Transition Metal Oxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2017, , .	0.0	0
95	Elucidating the Pre-Oxygen Evolution Surface Chemistry on Ruthenium Dioxide Surfaces. ECS Meeting Abstracts, 2017, , .	0.0	0
96	Oxygen Reduction Reaction Catalytic Sites on Carbon-Coated Fe3C Catalyst. ECS Meeting Abstracts, 2017, , .	0.0	0
97	Towards Identifying the Active Sites on Oriented Ruthenium Dioxide Surfaces in Catalyzing Oxygen Evolution. ECS Meeting Abstracts, 2018, , .	0.0	0
98	Design of Rutile Oxide Electrocatalysts for Selective Reduction of CO2 into Liquid Fuels. ECS Meeting Abstracts, 2018, , .	0.0	0
99	Understanding and Tailoring the Performance of Transition Metal Oxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2018, , .	0.0	0
100	CO₂ Activation at Au(110)-Water Interfaces: An Ab Initio Molecular Dynamics Study. ECS Meeting Abstracts, 2022, MA2022-01, 2098-2098.	0.0	0
101	Surface Properties of Graphite for Electrocatalysis of Vanadium Redox Reactions. ECS Meeting Abstracts, 2022, MA2022-01, 2037-2037.	0.0	0