Heine A Hansen

List of Publications by Citations

85 papers	11,799 citations	40 h-index	105 g-index
105 ext. papers	13,673 ext. citations	8 avg, IF	6.38 L-index

#	Paper	IF	Citations
85	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. *ChemCatChem*, **2011**, 3, 1159-1165	5.2	2321
84	Alloys of platinum and early transition metals as oxygen reduction electrocatalysts. *Nature Chemistry*, **2009**, 1, 552-6	17.6	2287
83	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. *Journal of Physics Condensed Matter*, **2010**, 22, 253202	1.8	1092
82	Understanding Trends in the Electrocatalytic Activity of Metals and Enzymes for CO2 Reduction to CO. *Journal of Physical Chemistry Letters*, **2013**, 4, 388-92	6.4	485
81	Universality in Oxygen Reduction Electrocatalysis on Metal Surfaces. *ACS Catalysis*, **2012**, 2, 1654-1660	13.1	360
80	Surface Pourbaix diagrams and oxygen reduction activity of Pt, Ag and Ni(111) surfaces studied by DFT. *Physical Chemistry Chemical Physics*, **2008**, 10, 3722-30	3.6	351
79	Trends in electrochemical CO2 reduction activity for open and close-packed metal surfaces. *Physical Chemistry Chemical Physics*, **2014**, 16, 4720-7	3.6	284
78	Direct observation of the oxygenated species during oxygen reduction on a platinum fuel cell cathode. *Nature Communications*, **2013**, 4,	17.4	261
77	Scaling relationships for adsorption energies on transition metal oxide, sulfide, and nitride surfaces. *Angewandte Chemie - International Edition*, **2008**, 47, 4683-6	16.4	260
76	Electrochemical chlorine evolution at rutile oxide (110) surfaces. *Physical Chemistry Chemical Physics*, **2010**, 12, 283-90	3.6	244
75	Unifying Kinetic and Thermodynamic Analysis of 2 e□ and 4 e□ Reduction of Oxygen on Metal Surfaces. *Journal of Physical Chemistry C*, **2014**, 118, 6706-6718	3.8	227
74	Unifying the 2e(-) and 4e(-) Reduction of Oxygen on Metal Surfaces. *Journal of Physical Chemistry Letters*, **2012**, 3, 2948-51	6.4	206
73	Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO2 Reduction. *ChemCatChem*, **2014**, 6, 1899-1905	5.2	194
72	Method for locating low-energy solutions within DFT+U. *Physical Review B*, **2010**, 82,	3.3	187
71	Towards identifying the active sites on RuO2(110) in catalyzing oxygen evolution. *Energy and Environmental Science*, **2017**, 10, 2626-2637	35.4	185
70	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 49-70	3.6	171
69	Orientation-Dependent Oxygen Evolution on RuO2 without Lattice Exchange. *ACS Energy Letters*, **2017**, 2, 876-881	20.1	165

68	The Pt(111)/electrolyte interface under oxygen reduction reaction conditions: an electrochemical impedance spectroscopy study. *Langmuir*, **2011**, 27, 2058-66	4	157
67	Identifying systematic DFT errors in catalytic reactions. *Catalysis Science and Technology*, **2015**, 5, 4946-4949	5.5	113
66	Synthesis of thin film AuPd alloys and their investigation for electrocatalytic CO2 reduction. *Journal of Materials Chemistry A*, **2015**, 3, 20185-20194	13	101
65	Bifunctional alloys for the electroreduction of CO2 and CO. *Physical Chemistry Chemical Physics*, **2016**, 18, 9194-201	3.6	101
64	Selective Electrochemical Generation of Hydrogen Peroxide from Water Oxidation. *Journal of Physical Chemistry Letters*, **2015**, 6, 4224-8	6.4	96
63	Opportunities and challenges in the electrocatalysis of CO2 and CO reduction using bifunctional surfaces: A theoretical and experimental study of Au□d alloys. *Journal of Catalysis*, **2016**, 343, 215-231	7.3	96
62	Mechanistic Pathway in the Electrochemical Reduction of CO2 on RuO2. *ACS Catalysis*, **2015**, 5, 4075-4081	13.1	95
61	Functional Independent Scaling Relation for ORR/OER Catalysts. *Journal of Physical Chemistry C*, **2016**, 120, 24910-24916	3.8	86
60	Formation energies of rutile metal dioxides using density functional theory. *Physical Review B*, **2009** , 79,	3.3	82
59	Elucidating the activity of stepped Pt single crystals for oxygen reduction. *Physical Chemistry Chemical Physics*, **2014**, 16, 13625-9	3.6	79
58	Density functional theory based screening of ternary alkali-transition metal borohydrides: a computational material design project. *Journal of Chemical Physics*, **2009**, 131, 014101	3.9	74
57	Modeling CO2 reduction on Pt(111). *Physical Chemistry Chemical Physics*, **2013**, 15, 7114-22	3.6	72
56	Electrochemical reduction of CO2 on compositionally variant Au-Pt bimetallic thin films. *Nano Energy*, **2017**, 42, 51-57	17.1	64
55	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	3.8	64
54	Kinetics and Thermodynamics of H2O Dissociation on Reduced CeO2(111). *Journal of Physical Chemistry C*, **2014**, 118, 27402-27414	3.8	58
53	2D transition metal□CNQ sheets as bifunctional single-atom catalysts for oxygen reduction and evolution reaction (ORR/OER). *Journal of Catalysis*, **2019**, 370, 378-384	7.3	57
52	OH formation and H adsorption at the liquid water-Pt(111) interface. *Chemical Science*, **2018**, 9, 6912-6921	9.4	57
51	DFT study of stabilization effects on N-doped graphene for ORR catalysis. *Catalysis Today*, **2018**, 312, 118-125	5.3	54

50	NiFeS Cubanes in CO2 Reduction Electrocatalysis: A DFT Study. *ACS Catalysis*, **2013**, 3, 2640-2643	13.1	53
49	A DFT-based genetic algorithm search for AuCu nanoalloy electrocatalysts for CO reduction. *Physical Chemistry Chemical Physics*, **2015**, 17, 28270-6	3.6	50
48	Volcano Relation for the Deacon Process over Transition-Metal Oxides. *ChemCatChem*, **2010**, 2, 98-102	5.2	48
47	Cation insertion to break the activity/stability relationship for highly active oxygen evolution reaction catalyst. *Nature Communications*, **2020**, 11, 1378	17.4	43
46	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	13.1	41
45	Comparative DFT+U and HSE Study of the Oxygen Evolution Electrocatalysis on Perovskite Oxides. *Journal of Physical Chemistry C*, **2018**, 122, 1135-1147	3.8	39
44	Pt Skin Versus Pt Skeleton Structures of Pt3Sc as Electrocatalysts for Oxygen Reduction. *Topics in Catalysis*, **2014**, 57, 245-254	2.3	36
43	First principles investigation of the activity of thin film Pt, Pd and Au surface alloys for oxygen reduction. *Physical Chemistry Chemical Physics*, **2015**, 17, 11647-57	3.6	35
42	Giant onsite electronic entropy enhances the performance of ceria for water splitting. *Nature Communications*, **2017**, 8, 285	17.4	35
41	Universality in Nonaqueous Alkali Oxygen Reduction on Metal Surfaces: Implications for LiO2 and NaO2 Batteries. *ACS Energy Letters*, **2016**, 1, 162-168	20.1	35
40	DFT Study of the Oxygen Reduction Reaction on Carbon-Coated Iron and Iron Carbide. *ACS Catalysis*, **2018**, 8, 10521-10529	13.1	33
39	First principles investigation of zinc-anode dissolution in zinc-air batteries. *Physical Chemistry Chemical Physics*, **2013**, 15, 6416-21	3.6	31
38	Enhanced Oxygen Reduction Activity by Selective Anion Adsorption on Non-Precious-Metal Catalysts. *ACS Catalysis*, **2018**, 8, 7104-7112	13.1	29
37	Ti atoms in Ru0.3Ti0.7O2 mixed oxides form active and selective sites for electrochemical chlorine evolution. *Electrochimica Acta*, **2014**, 146, 733-740	6.7	29
36	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	2.5	29
35	Unifying Solution and Surface Electrochemistry: Limitations and Opportunities in Surface Electrocatalysis. *Topics in Catalysis*, **2014**, 57, 215-221	2.3	28
34	Descriptors and Thermodynamic Limitations of Electrocatalytic Carbon Dioxide Reduction on Rutile Oxide Surfaces. *ChemSusChem*, **2016**, 9, 3230-3243	8.3	27
33	Computational Screening of Doped MnO Catalysts for the Oxygen Evolution Reaction. *ChemSusChem*, **2018**, 11, 629-637	8.3	27

32	Reducing Systematic Errors in Oxide Species with Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2015**, 119, 17596-17601	3.8	25
31	Using microkinetic analysis to search for novel anhydrous formaldehyde production catalysts. *Surface Science*, **2015**, 641, 105-111	1.8	22
30	Combined DFT and Differential Electrochemical Mass Spectrometry Investigation of the Effect of Dopants in Secondary Zinc-Air Batteries. *ChemSusChem*, **2018**, 11, 1933-1941	8.3	20
29	Electroreduction of Methanediol on Copper. *Catalysis Letters*, **2013**, 143, 631-635	2.8	19
28	Mechanism of Water Splitting on Gadolinium-Doped CeO2(111): A DFT + U Study. *Journal of Physical Chemistry C*, **2019**, 123, 5507-5517	3.8	18
27	Decoupling strain and ligand effects in ternary nanoparticles for improved ORR electrocatalysis. *Physical Chemistry Chemical Physics*, **2016**, 18, 24737-45	3.6	18
26	Energy-entropy competition in cation-hydroxyl interactions at the liquid water-Pt(111) interface. *Chemical Communications*, **2020**, 56, 427-430	5.8	17
25	Improving the Activity of M-N Catalysts for the Oxygen Reduction Reaction by Electrolyte Adsorption. *ChemSusChem*, **2019**, 12, 5133-5141	8.3	16
24	Facet-dependent electrocatalytic water splitting reaction on CeO2: A DFT□+□U study. *Journal of Catalysis*, **2020**, 388, 1-10	7.3	14
23	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	13	14
22	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	7.3	14
21	Improved Electrocatalytic Water Splitting Reaction on CeO2(111) by Strain Engineering: A DFT+U Study. *ACS Catalysis*, **2019**, 9, 4853-4861	13.1	13
20	N-Doped Graphene Supported on Metal-Iron Carbide as a Catalyst for the Oxygen Reduction Reaction: Density Functional Theory Study. *ChemSusChem*, **2020**, 13, 996-1005	8.3	13
19	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	3.6	11
18	Role of CO* as a Spectator in CO2 Electroreduction on RuO2. *Journal of Physical Chemistry C*, **2017**, 121, 18333-18343	3.8	11
17	Volcano Relations for Oxidation of Hydrogen Halides over Rutile Oxide Surfaces. *ChemCatChem*, **2012**, 4, 1856-1861	5.2	11
16	Rate enhancement in microfabricated chemical reactors under fast forced temperature oscillations. *Catalysis Communications*, **2006**, 7, 272-275	3.2	11
15	Acid-Stable and Active M□□□ Catalysts for the Oxygen Reduction Reaction: The Role of Local Structure. *ACS Catalysis*,13102-13118	13.1	11

14	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	6.4	11
13	Computational Study of Nb-Doped-SnO2/Pt Interfaces: Dopant Segregation, Electronic Transport, and Catalytic Properties. *Chemistry of Materials*, **2017**, 29, 1641-1649	9.6	10
12	Electrochemical Reduction of CO2 on IrxRu(1−x)O2(110) Surfaces. *ACS Catalysis*, **2017**, 7, 8502-8513	13.1	9
11	Ternary ruthenium complex hydrides for ammonia synthesis via the associative mechanism. *Nature Catalysis*, **2021**, 4, 959-967	36.5	9
10	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	7.3	7
9	The Role of Oxygenic Groups and sp Carbon Hybridization in Activated Graphite Electrodes for Vanadium Redox Flow Batteries. *ChemSusChem*, **2021**, 14, 3945-3952	8.3	5
8	CO activation at Au(110)-water interfaces: An ab initio molecular dynamics study. *Journal of Chemical Physics*, **2021**, 155, 134703	3.9	5
7	DFT + U Study of Strain-Engineered CO2 Reduction on a CeO2−x (111) Facet. *Journal of Physical Chemistry C*, **2021**, 125, 14221-14227	3.8	4
6	DFT+U study of CO2 reduction and CO oxidation on a reconstructed CeO2(110) facet. *Materials Today Advances*, **2020**, 8, 100111	7.4	3
5	Layered double hydroxides as advanced tracks to promote ionic conductivity in metal borohydride. *Materials Chemistry Frontiers*,	7.8	2
4	The role of nitrogen and sulfur dual coordination of cobalt in Co-N4−xSx/C single atom catalysts in the oxygen reduction reaction. *Sustainable Energy and Fuels*,	5.8	1
3	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	7.3	1
2	Degradation of polybenzimidazole in alkaline solution with First-Principles Modelling. *Electrochimica Acta*, **2021**, 139329	6.7	0
1	Formation of a Complex Active Center by Ba2RuH6 for Nondissociative Dinitrogen Activation and Ammonia Formation. *ACS Catalysis*, **2022**, 12, 4194-4202	13.1	0