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	Structure and energetics of liquid waterâ€“hydroxyl layers on Pt(111). Physical Chemistry Chemical Physics, 2022, 24, 9885-9890.	1.3	8
2	Formation of a Complex Active Center by Ba₂RuH₆ for Nondissociative Dinitrogen Activation and Ammonia Formation. ACS Catalysis, 2022, 12, 4194-4202.	5.5	15
3	Metalâ€Doped PdH(111) Catalysts for CO₂ Reduction. ChemSusChem, 2022, 15, .	3.6	7
4	Unfolding the structural stability of nanoalloys via symmetry-constrained genetic algorithm and neural network potential. Npj Computational Materials, 2022, 8, .	3.5	9
5	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
6	CO₂ Activation at Au(110)-Water Interfaces: An Ab Initio Molecular Dynamics Study. ECS Meeting Abstracts, 2022, MA2022-01, 2098-2098.	0.0	0
7	Surface Properties of Graphite for Electrocatalysis of Vanadium Redox Reactions. ECS Meeting Abstracts, 2022, MA2022-01, 2037-2037.	0.0	0
8	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
9	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
10	Layered double hydroxides as advanced tracks to promote ionic conductivity in metal borohydride. Materials Chemistry Frontiers, 2021, 5, 4989-4996.	3.2	6
11	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
12	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
13	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
14	Degradation of polybenzimidazole in alkaline solution with first-principles Modeling. Electrochimica Acta, 2021, 398, 139329.	2.6	5
15	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
16	CO2 activation at Au(110)â€“water interfaces: An ab initio molecular dynamics study. Journal of Chemical Physics, 2021, 155, 134703.	1.2	13
17	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
18	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

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19	Ternary ruthenium complex hydrides for ammonia synthesis via the associative mechanism. Nature Catalysis, 2021, 4, 959-967.	16.1	67
20	Energyâ€“entropy competition in cationâ€“hydroxyl interactions at the liquid waterâ€“Pt(111) interface. Chemical Communications, 2020, 56, 427-430.	2.2	25
21	Nâ€Doped 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
22	DFT+U study of CO2 reduction and CO oxidation on a reconstructed CeO2â˜(110) facet. Materials Today Advances, 2020, 8, 100111.	2.5	8
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.	5.2	29
24	Facet-dependent electrocatalytic water splitting reaction on CeO2: A DFTÂ+ÂU study. Journal of Catalysis, 2020, 388, 1-10.	3.1	32
25	Cation insertion to break the activity/stability relationship for highly active oxygen evolution reaction catalyst. Nature Communications, 2020, 11, 1378.	5.8	79
26	Improving the Activity of Mâ˜N₄ Catalysts for the Oxygen Reduction Reaction by Electrolyte Adsorption. ChemSusChem, 2019, 12, 5133-5141.	3.6	33
27	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
28	Improved Electrocatalytic Water Splitting Reaction on CeO₂(111) by Strain Engineering: A DFT+U Study. ACS Catalysis, 2019, 9, 4853-4861.	5.5	37
29	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
30	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
31	DFT study of stabilization effects on N-doped graphene for ORR catalysis. Catalysis Today, 2018, 312, 118-125.	2.2	81
32	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
33	Computational Screening of Doped Î±â€MnO₂ Catalysts for the Oxygen Evolution Reaction. ChemSusChem, 2018, 11, 629-637.	3.6	40
34	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
35	DFT Study of the Oxygen Reduction Reaction on Carbon-Coated Iron and Iron Carbide. ACS Catalysis, 2018, 8, 10521-10529.	5.5	46
36	OH formation and H₂ adsorption at the liquid waterâ€“Pt(111) interface. Chemical Science, 2018, 9, 6912-6921.	3.7	76

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37	Enhanced Oxygen Reduction Activity by Selective Anion Adsorption on Non-Precious-Metal Catalysts. ACS Catalysis, 2018, 8, 7104-7112.	5.5	53
38	Towards Identifying the Active Sites on Oriented Ruthenium Dioxide Surfaces in Catalyzing Oxygen Evolution. ECS Meeting Abstracts, 2018, , .	0.0	0
39	Design of Rutile Oxide Electrocatalysts for Selective Reduction of CO2 into Liquid Fuels. ECS Meeting Abstracts, 2018, , .	0.0	0
40	Understanding and Tailoring the Performance of Transition Metal Oxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2018, , .	0.0	0
41	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
42	Orientation-Dependent Oxygen Evolution on RuO₂ without Lattice Exchange. ACS Energy Letters, 2017, 2, 876-881.	8.8	251
43	Electrochemical Reduction of CO2 on IrxRu(1â€“x)O2(110) Surfaces. ACS Catalysis, 2017, 7, 8502-8513.	5.5	16
44	Electrochemical reduction of CO2 on compositionally variant Au-Pt bimetallic thin films. Nano Energy, 2017, 42, 51-57.	8.2	99
45	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
46	Role of CO* as a Spectator in CO2 Electroreduction on RuO2. Journal of Physical Chemistry C, 2017, 121, 18333-18343.	1.5	14
47	Giant onsite electronic entropy enhances the performance of ceria for water splitting. Nature Communications, 2017, 8, 285.	5.8	51
48	Towards identifying the active sites on RuO₂(110) in catalyzing oxygen evolution. Energy and Environmental Science, 2017, 10, 2626-2637.	15.6	278
49	Understanding and Tailoring the Performance of Transition Metal Oxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2017, , .	0.0	0
50	Elucidating the Pre-Oxygen Evolution Surface Chemistry on Ruthenium Dioxide Surfaces. ECS Meeting Abstracts, 2017, , .	0.0	0
51	Oxygen Reduction Reaction Catalytic Sites on Carbon-Coated Fe3C Catalyst. ECS Meeting Abstracts, 2017, , .	0.0	0
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	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
54	Decoupling strain and ligand effects in ternary nanoparticles for improved ORR electrocatalysis. Physical Chemistry Chemical Physics, 2016, 18, 24737-24745.	1.3	26

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55	Descriptors and Thermodynamic Limitations of Electrocatalytic Carbon Dioxide Reduction on Rutile Oxide Surfaces. ChemSusChem, 2016, 9, 3230-3243.	3.6	34
56	Functional Independent Scaling Relation for ORR/OER Catalysts. Journal of Physical Chemistry C, 2016, 120, 24910-24916.	1.5	119
57	Bifunctional alloys for the electroreduction of CO₂and CO. Physical Chemistry Chemical Physics, 2016, 18, 9194-9201.	1.3	127
58	DFT Studies of the Oxygen Reduction Reaction on Pristine and N-Doped Fe3C/Graphene Catalyst. ECS Meeting Abstracts, 2016, , .	0.0	0
59	Tailoring the Performance of Oxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2016, , .	0.0	0
60	ORR Activity of Pristine Graphite | Fe3c Interfaces. ECS Meeting Abstracts, 2016, , .	0.0	0
61	(Invited) Genetic Algorithms and DFT for Accelerated Design of Nanoalloys. ECS Meeting Abstracts, 2016, , .	0.0	0
62	Mechanistic Pathway in the Electrochemical Reduction of CO2 on RuO2. ACS Catalysis, 2015, 5, 4075-4081.	5.5	123
63	Using microkinetic analysis to search for novel anhydrous formaldehyde production catalysts. Surface Science, 2015, 641, 105-111.	0.8	25
64	Reducing Systematic Errors in Oxide Species with Density Functional Theory Calculations. Journal of Physical Chemistry C, 2015, 119, 17596-17601.	1.5	29
65	A DFT-based genetic algorithm search for AuCu nanoalloy electrocatalysts for CO₂ reduction. Physical Chemistry Chemical Physics, 2015, 17, 28270-28276.	1.3	65
66	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
67	Identifying systematic DFT errors in catalytic reactions. Catalysis Science and Technology, 2015, 5, 4946-4949.	2.1	144
68	Selective Electrochemical Generation of Hydrogen Peroxide from Water Oxidation. Journal of Physical Chemistry Letters, 2015, 6, 4224-4228.	2.1	142
69	Synthesis of thin film AuPd alloys and their investigation for electrocatalytic CO₂reduction. Journal of Materials Chemistry A, 2015, 3, 20185-20194.	5.2	116
70	Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO₂ Reduction. ChemCatChem, 2014, 6, 1899-1905.	1.8	255
71	Kinetics and Thermodynamics of H₂O Dissociation on Reduced CeO₂(111). Journal of Physical Chemistry C, 2014, 118, 27402-27414.	1.5	91
72	Elucidating the activity of stepped Pt single crystals for oxygen reduction. Physical Chemistry Chemical Physics, 2014, 16, 13625.	1.3	92

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73	Trends in electrochemical CO2 reduction activity for open and close-packed metal surfaces. Physical Chemistry Chemical Physics, 2014, 16, 4720.	1.3	375
74	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
75	Unifying Solution and Surface Electrochemistry: Limitations and Opportunities in Surface Electrocatalysis. Topics in Catalysis, 2014, 57, 215-221.	1.3	35
76	Pt Skin Versus Pt Skeleton Structures of Pt3Sc as Electrocatalysts for Oxygen Reduction. Topics in Catalysis, 2014, 57, 245-254.	1.3	47
77	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
78	Niâ€“Feâ€“S Cubanes in CO₂ Reduction Electrocatalysis: A DFT Study. ACS Catalysis, 2013, 3, 2640-2643.	5.5	68
79	Direct observation of the oxygenated species during oxygen reduction on a platinum fuel cell cathode. Nature Communications, 2013, 4, .	5.8	325
80	Electroreduction of Methanediol on Copper. Catalysis Letters, 2013, 143, 631-635.	1.4	21
81	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
82	Modeling CO2 reduction on Pt(111). Physical Chemistry Chemical Physics, 2013, 15, 7114.	1.3	80
83	First principles investigation of zinc-anode dissolution in zincâ€“air batteries. Physical Chemistry Chemical Physics, 2013, 15, 6416.	1.3	44
84	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
85	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
86	Volcano Relations for Oxidation of Hydrogen Halides over Rutile Oxide Surfaces. ChemCatChem, 2012, 4, 1856-1861.	1.8	11
87	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. Physical Chemistry Chemical Physics, 2012, 14, 49-70.	1.3	198
88	Universality in Oxygen Reduction Electrocatalysis on Metal Surfaces. ACS Catalysis, 2012, 2, 1654-1660.	5.5	456
89	The Pt(111)/Electrolyte Interface under Oxygen Reduction Reaction Conditions: An Electrochemical Impedance Spectroscopy Study. Langmuir, 2011, 27, 2058-2066.	1.6	170
90	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. ChemCatChem, 2011, 3, 1159-1165.	1.8	3,208

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91	Volcano Relation for the Deacon Process over Transitionâ€Metal Oxides. ChemCatChem, 2010, 2, 98-102.	1.8	49
92	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
93	Electrochemical chlorine evolution at rutile oxide (110) surfaces. Physical Chemistry Chemical Physics, 2010, 12, 283-290.	1.3	317
94	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
95	Formation energies of rutile metal dioxides using density functional theory. Physical Review B, 2009, 79, .	1.1	87
96	Alloys of platinum and early transition metals as oxygen reduction electrocatalysts. Nature Chemistry, 2009, 1, 552-556.	6.6	2,716
97	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
98	Scaling Relationships for Adsorption Energies on Transition Metal Oxide, Sulfide, and Nitride Surfaces. Angewandte Chemie - International Edition, 2008, 47, 4683-4686.	7.2	301
99	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
100	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
101	Rate enhancement in microfabricated chemical reactors under fast forced temperature oscillations. Catalysis Communications, 2006, 7, 272-275.	1.6	13