Samira Siahrostami

List of Publications by Citations

77 papers	7,625 citations	39 h-index	86 g-index
86 ext. papers	10,388 ext. citations	12 avg, IF	6.44 L-index

#	Paper	IF	Citations
77	Understanding Catalytic Activity Trends in the Oxygen Reduction Reaction. *Chemical Reviews*, **2018**, 118, 2302-2312	68.1	908
76	Enabling direct H2O2 production through rational electrocatalyst design. *Nature Materials*, **2013**, 12, 1137-43	27	649
75	High-efficiency oxygen reduction to hydrogen peroxide catalysed by oxidized carbon materials. *Nature Catalysis*, **2018**, 1, 156-162	36.5	632
74	Isolated Ni single atoms in graphene nanosheets for high-performance CO2 reduction. *Energy and Environmental Science*, **2018**, 11, 893-903	35.4	580
73	The oxygen reduction reaction mechanism on Pt(111) from density functional theory calculations. *Electrochimica Acta*, **2010**, 55, 7975-7981	6.7	387
72	Trends in the electrochemical synthesis of H2O2: enhancing activity and selectivity by electrocatalytic site engineering. *Nano Letters*, **2014**, 14, 1603-8	11.5	352
71	Highly selective oxygen reduction to hydrogen peroxide on transition metal single atom coordination. *Nature Communications*, **2019**, 10, 3997	17.4	264
70	Transition-Metal Single Atoms in a Graphene Shell as Active Centers for Highly Efficient Artificial Photosynthesis. *CheM*, **2017**, 3, 950-960	16.2	249
69	Beyond the top of the volcano? A unified approach to electrocatalytic oxygen reduction and oxygen evolution. *Nano Energy*, **2016**, 29, 126-135	17.1	195
68	Understanding activity trends in electrochemical water oxidation to form hydrogen peroxide. *Nature Communications*, **2017**, 8, 701	17.4	193
67	Designing Boron Nitride Islands in Carbon Materials for Efficient Electrochemical Synthesis of Hydrogen Peroxide. *Journal of the American Chemical Society*, **2018**, 140, 7851-7859	16.4	184
66	Introducing Fe into Nickel-Iron Layered Double Hydroxide: Local Structure Modulated Water Oxidation Activity. *Angewandte Chemie - International Edition*, **2018**, 57, 9392-9396	16.4	181
65	Defective Carbon-Based Materials for the Electrochemical Synthesis of Hydrogen Peroxide. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 311-317	8.3	153
64	One- or Two-Electron Water Oxidation, Hydroxyl Radical, or HO Evolution. *Journal of Physical Chemistry Letters*, **2017**, 8, 1157-1160	6.4	142
63	Monocopper Active Site for Partial Methane Oxidation in Cu-Exchanged 8MR Zeolites. *ACS Catalysis* , **2016**, 6, 6531-6536	13.1	136
62	Electrochemical ammonia synthesis via nitrate reduction on Fe single atom catalyst. *Nature Communications*, **2021**, 12, 2870	17.4	136
61	Cation-exchanged zeolites for the selective oxidation of methane to methanol. *Catalysis Science and Technology*, **2018**, 8, 114-123	5.5	110

60	Building and identifying highly active oxygenated groups in carbon materials for oxygen reduction to HO. *Nature Communications*, **2020**, 11, 2209	17.4	107
59	Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide. *Nature Catalysis*, **2020**, 3, 125-134	36.5	106
58	Development of a reactor with carbon catalysts for modular-scale, low-cost electrochemical generation of H2O2. *Reaction Chemistry and Engineering*, **2017**, 2, 239-245	4.9	100
57	ZnO As an Active and Selective Catalyst for Electrochemical Water Oxidation to Hydrogen Peroxide. *ACS Catalysis*, **2019**, 9, 4593-4599	13.1	95
56	A Review on Challenges and Successes in Atomic-Scale Design of Catalysts for Electrochemical Synthesis of Hydrogen Peroxide. *ACS Catalysis*, **2020**, 10, 7495-7511	13.1	95
55	Effects of redox-active interlayer anions on the oxygen evolution reactivity of NiFe-layered double hydroxide nanosheets. *Nano Research*, **2018**, 11, 1358-1368	10	93
54	Promoting HO production via 2-electron oxygen reduction by coordinating partially oxidized Pd with defect carbon. *Nature Communications*, **2020**, 11, 2178	17.4	79
53	Enhancing Catalytic Activity of MoS2 Basal Plane S-Vacancy by Co Cluster Addition. *ACS Energy Letters*, **2018**, 3, 2685-2693	20.1	79
52	CaSnO3: An Electrocatalyst for Two-Electron Water Oxidation Reaction to Form H2O2. *ACS Energy Letters*, **2019**, 4, 352-357	20.1	77
51	Selective and Efficient Gd-Doped BiVO4 Photoanode for Two-Electron Water Oxidation to H2O2. *ACS Energy Letters*, **2019**, 4, 720-728	20.1	76
50	Theoretical Investigations into Defected Graphene for Electrochemical Reduction of CO2. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 11080-11085	8.3	68
49	A Porphyrinic Zirconium Metal-Organic Framework for Oxygen Reduction Reaction: Tailoring the Spacing between Active-Sites through Chain-Based Inorganic Building Units. *Journal of the American Chemical Society*, **2020**, 142, 15386-15395	16.4	65
48	Light-Driven BiVO4□ Fuel Cell with Simultaneous Production of H2O2. *Advanced Energy Materials*, **2018**, 8, 1801158	21.8	64
47	Introducing Fe2+ into Nickel□ron Layered Double Hydroxide: Local Structure Modulated Water Oxidation Activity. *Angewandte Chemie*, **2018**, 130, 9536-9540	3.6	61
46	Influence of Adsorbed Water on the Oxygen Evolution Reaction on Oxides. *Journal of Physical Chemistry C*, **2015**, 119, 1032-1037	3.8	55
45	Mechanochemistry for ammonia synthesis under mild conditions. *Nature Nanotechnology*, **2021**, 16, 325-330	38.7	51
44	High-performance oxygen reduction and evolution carbon catalysis: From mechanistic studies to device integration. *Nano Research*, **2017**, 10, 1163-1177	10	50
43	Precious Metal-Free Nickel Nitride Catalyst for the Oxygen Reduction Reaction. *ACS Applied Materials & Interfaces*, **2019**, 11, 26863-26871	9.5	47

42	Electrochemical Synthesis of H2O2 by Two-Electron Water Oxidation Reaction. *CheM*, **2021**, 7, 38-63	16.2	45
41	Catalytic hydrogenation of CC and CO in unsaturated fatty acid methyl esters. *Catalysis Science and Technology*, **2014**, 4, 2427-2444	5.5	42
40	Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene. *ACS Central Science*, **2017**, 3, 1286-1293	16.8	41
39	Two-Dimensional Materials as Catalysts for Energy Conversion. *Catalysis Letters*, **2016**, 146, 1917-1921	2.8	39
38	Theoretical Approaches to Describing the Oxygen Reduction Reaction Activity of Single-Atom Catalysts. *Journal of Physical Chemistry C*, **2018**, 122, 29307-29318	3.8	39
37	Single Metal Atoms Anchored in Two-Dimensional Materials: Bifunctional Catalysts for Fuel Cell Applications. *ChemCatChem*, **2018**, 10, 3034-3039	5.2	37
36	Structural and Energetic Trends of Ethylene Hydrogenation over Transition Metal Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 995-1003	3.8	37
35	Ultrathin Cobalt Oxide Overlayer Promotes Catalytic Activity of Cobalt Nitride for the Oxygen Reduction Reaction. *Journal of Physical Chemistry C*, **2018**, 122, 4783-4791	3.8	36
34	Nature of Lone-Pair-Surface Bonds and Their Scaling Relations. *Inorganic Chemistry*, **2018**, 57, 7222-7238	5.1	35
33	Tandem cathode for proton exchange membrane fuel cells. *Physical Chemistry Chemical Physics*, **2013**, 15, 9326-34	3.6	34
32	A review on electrocatalytic oxidation of methane to oxygenates. *Journal of Materials Chemistry A*, **2020**, 8, 15575-15590	13	33
31	First principles investigation of zinc-anode dissolution in zinc-air batteries. *Physical Chemistry Chemical Physics*, **2013**, 15, 6416-21	3.6	31
30	H(2) production through electro-oxidation of SO(2): identifying the fundamental limitations. *Physical Chemistry Chemical Physics*, **2014**, 16, 9572-9	3.6	27
29	Electron affinity and redox potential of tetrafluoro-p-benzoquinone: A theoretical study. *Journal of Fluorine Chemistry*, **2008**, 129, 222-225	2.1	22
28	Copper Silver Thin Films with Metastable Miscibility for Oxygen Reduction Electrocatalysis in Alkaline Electrolytes. *ACS Applied Energy Materials*, **2018**, 1, 1990-1999	6.1	21
27	Improved Oxygen Reduction Reaction Activity of Nanostructured CoS2 through Electrochemical Tuning. *ACS Applied Energy Materials*, **2019**, 2, 8605-8614	6.1	21
26	Calculation of two-electron reduction potentials for some quinone derivatives in aqueous solution using M□ller□Plesset perturbation theory. *Computational and Theoretical Chemistry*, **2006**, 759, 245-247		20
25	Orbital graph convolutional neural network for material property prediction. *Physical Review Materials*, **2020**, 4,	3.2	19

24	Ligand-Engineered Metal□Organic Frameworks for Electrochemical Reduction of Carbon Dioxide to Carbon Monoxide. *ACS Catalysis*, **2021**, 11, 7350-7357	13.1	17
23	Noble metal supported hexagonal boron nitride for the oxygen reduction reaction: a DFT study. *Nanoscale Advances*, **2019**, 1, 132-139	5.1	16
22	Exploring Scaling Relations for Chemisorption Energies on Transition-Metal-Exchanged Zeolites ZSM-22 and ZSM-5. *ChemCatChem*, **2016**, 8, 767-772	5.2	16
21	Circumventing Scaling Relations in Oxygen Electrochemistry Using Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2020**, 11, 10029-10036	6.4	16
20	In Situ X-Ray Absorption Spectroscopy Disentangles the Roles of Copper and Silver in a Bimetallic Catalyst for the Oxygen Reduction Reaction. *Chemistry of Materials*, **2020**, 32, 1819-1827	9.6	15
19	Application of Density Functional Theory for evaluation of standard two-electron reduction potentials in some quinone derivatives. *Computational and Theoretical Chemistry*, **2008**, 870, 10-14		15
18	Prediction of Stable and Active (Oxy-Hydro) Oxide Nanoislands on Noble-Metal Supports for Electrochemical Oxygen Reduction Reaction. *ACS Applied Materials & Interfaces*, **2019**, 11, 2006-2013	9.5	14
17	An insight into microscopic properties of aprotic ionic liquids: A DFT study. *Computational and Theoretical Chemistry*, **2010**, 955, 47-52		13
16	Coproduction of hydrogen and lactic acid from glucose photocatalysis on band-engineered ZnCdS homojunction. *IScience*, **2021**, 24, 102109	6.1	13
15	Development of Fukui Function Based Descriptors for a Machine Learning Study of CO2 Reduction. *Journal of Physical Chemistry C*, **2020**, 124, 10079-10084	3.8	12
14	Trends in Adsorption Energies of the Oxygenated Species on Single Platinum Atom Embedded in Carbon Nanotubes. *Catalysis Letters*, **2017**, 147, 2689-2696	2.8	10
13	Activity and Selectivity for O2 Reduction to H2O2 on Transition Metal Surfaces. *ECS Transactions*, **2013**, 58, 53-62	1	9
12	High-Throughput Electron Diffraction Reveals a Hidden Novel Metal-Organic Framework for Electrocatalysis. *Angewandte Chemie - International Edition*, **2021**, 60, 11391-11397	16.4	9
11	Ternary cobalt□iron sulfide as a robust electrocatalyst for water oxidation: A dual effect from surface evolution and metal doping. *Applied Surface Science*, **2021**, 542, 148681	6.7	9
10	Effect of Adventitious Carbon on Pit Formation of Monolayer MoS. *Advanced Materials*, **2020**, 32, e2003020	24	5
9	Designing Carbon-Based Materials for Efficient Electrochemical Reduction of CO2. *Industrial & Engineering Chemistry Research*, **2019**, 58, 879-885	3.9	5
8	Exploring the Effect of Gold Support on the Oxygen Reduction Reaction Activity of Metal Porphycenes. *ChemCatChem*, **2018**, 10, 5505-5510	5.2	4
7	Two-Dimensional Metal□Organic Frameworks with Unique Oriented Layers for Oxygen Reduction Reaction: Tailoring the Activity through Exposed Crystal Facets. *CCS Chemistry*,1-10	7.2	3

6	Elaborating Nitrogen and Oxygen Dopants Configurations within Graphene Electrocatalysts for Two-Electron Oxygen Reduction320-328		2
5	Heteroatom-Doped Transition Metal Nitrides for CO Electrochemical Reduction: A Density Functional Theory Screening Study. *Journal of Physical Chemistry C*, **2020**, 124, 26344-26351	3.8	2
4	The role of Pt in MoC on the water-gas shift reaction at low temperatures. *Joule*, **2021**, 5, 521-523	27.8	2
3	High-Performance Zinc-Air Batteries Based on Bifunctional Hierarchically Porous Nitrogen-Doped Carbon. *Small*, **2021**, e2105928	11	2
2	SnO2-supported single metal atoms: a bifunctional catalyst for the electrochemical synthesis of H2O2. *Journal of Materials Chemistry A*,	13	1
1	High-Throughput Electron Diffraction Reveals a Hidden Novel Metal Organic Framework for Electrocatalysis. *Angewandte Chemie*, **2021**, 133, 11492-11498	3.6	0