# Samira Siahrostami

List of Publications by Year
in descending order



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|---|---|---|---|
| 82 papers | 13,245 citations | 50170 46 h-index | 62479 80 g-index |
| 86 all docs | 86 docs citations | 86 times ranked | 11137 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Understanding Catalytic Activity Trends in the Oxygen Reduction Reaction. Chemical Reviews, 2018, 118, 2302-2312. | 23.0 | 1,666 |
| 2 | High-efficiency oxygen reduction to hydrogen peroxide catalysed by oxidized carbon materials. Nature Catalysis, 2018, 1, 156-162. | 16.1 | 1,120 |
| 3 | Enabling direct H2O2 production through rational electrocatalyst design. Nature Materials, 2013, 12, 1137-1143. | 13.3 | 1,031 |
| 4 | Isolated Ni single atoms in graphene nanosheets for high-performance CO<sub>2</sub> reduction. Energy and Environmental Science, 2018, 11, 893-903. | 15.6 | 811 |
| 5 | Electrochemical ammonia synthesis via nitrate reduction on Fe single atom catalyst. Nature Communications, 2021, 12, 2870. | 5.8 | 605 |
| 6 | Highly selective oxygen reduction to hydrogen peroxide on transition metal single atom coordination. Nature Communications, 2019, 10, 3997. | 5.8 | 528 |
| 7 | Trends in the Electrochemical Synthesis of H<sub>2</sub>O<sub>2</sub>: Enhancing Activity and Selectivity by Electrocatalytic Site Engineering. Nano Letters, 2014, 14, 1603-1608. | 4.5 | 521 |
| 8 | The oxygen reduction reaction mechanism on Pt(111) from density functional theory calculations. Electrochimica Acta, 2010, 55, 7975-7981. | 2.6 | 491 |
| 9 | Understanding activity trends in electrochemical water oxidation to form hydrogen peroxide. Nature Communications, 2017, 8, 701. | 5.8 | 333 |
| 10 | Transition-Metal Single Atoms in a Graphene Shell as Active Centers for Highly Efficient Artificial Photosynthesis. CheM, 2017, 3, 950-960. | 5.8 | 326 |
| 11 | Designing Boron Nitride Islands in Carbon Materials for Efficient Electrochemical Synthesis of Hydrogen Peroxide. Journal of the American Chemical Society, 2018, 140, 7851-7859. | 6.6 | 310 |
| 12 | Introducing Fe<sup>2+</sup> into Nickelâ€“Iron Layered Double Hydroxide: Local Structure Modulated Water Oxidation Activity. Angewandte Chemie - International Edition, 2018, 57, 9392-9396. | 7.2 | 284 |
| 13 | Building and identifying highly active oxygenated groups in carbon materials for oxygen reduction to H2O2. Nature Communications, 2020, 11, 2209. | 5.8 | 281 |
| 14 | A Review on Challenges and Successes in Atomic-Scale Design of Catalysts for Electrochemical Synthesis of Hydrogen Peroxide. ACS Catalysis, 2020, 10, 7495-7511. | 5.5 | 254 |
| 15 | Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide. Nature Catalysis, 2020, 3, 125-134. | 16.1 | 252 |
| 16 | Beyond the top of the volcano? â€“ A unified approach to electrocatalytic oxygen reduction and oxygen evolution. Nano Energy, 2016, 29, 126-135. | 8.2 | 248 |
| 17 | Defective Carbon-Based Materials for the Electrochemical Synthesis of Hydrogen Peroxide. ACS Sustainable Chemistry and Engineering, 2018, 6, 311-317. | 3.2 | 236 |
| 18 | One- or Two-Electron Water Oxidation, Hydroxyl Radical, or H<sub>2</sub>O<sub>2</sub> Evolution. Journal of Physical Chemistry Letters, 2017, 8, 1157-1160. | 2.1 | 234 |

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|---|---|---|---|
| 19 | Promoting H2O2 production via 2-electron oxygen reduction by coordinating partially oxidized Pd with defect carbon. Nature Communications, 2020, 11, 2178. | 5.8 | 209 |
| 20 | ZnO As an Active and Selective Catalyst for Electrochemical Water Oxidation to Hydrogen Peroxide. ACS Catalysis, 2019, 9, 4593-4599. | 5.5 | 176 |
| 21 | Monocopper Active Site for Partial Methane Oxidation in Cu-Exchanged 8MR Zeolites. ACS Catalysis, 2016, 6, 6531-6536. | 5.5 | 173 |
| 22 | Selective and Efficient Gd-Doped BiVO<sub>4</sub> Photoanode for Two-Electron Water Oxidation to H<sub>2</sub>O<sub>2</sub>. ACS Energy Letters, 2019, 4, 720-728. | 8.8 | 165 |
| 23 | Development of a reactor with carbon catalysts for modular-scale, low-cost electrochemical generation of H<sub>2</sub>O<sub>2</sub>. Reaction Chemistry and Engineering, 2017, 2, 239-245. | 1.9 | 157 |
| 24 | Electrochemical Synthesis of H2O2 by Two-Electron Water Oxidation Reaction. CheM, 2021, 7, 38-63. | 5.8 | 155 |
| 25 | CaSnO<sub>3</sub>: An Electrocatalyst for Two-Electron Water Oxidation Reaction to Form H<sub>2</sub>O<sub>2</sub>. ACS Energy Letters, 2019, 4, 352-357. | 8.8 | 148 |
| 26 | Mechanochemistry for ammonia synthesis under mild conditions. Nature Nanotechnology, 2021, 16, 325-330. | 15.6 | 141 |
| 27 | A Porphyrinic Zirconium Metalâ€“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. | 6.6 | 139 |
| 28 | Cation-exchanged zeolites for the selective oxidation of methane to methanol. Catalysis Science and Technology, 2018, 8, 114-123. | 2.1 | 135 |
| 29 | Effects of redox-active interlayer anions on the oxygen evolution reactivity of NiFe-layered double hydroxide nanosheets. Nano Research, 2018, 11, 1358-1368. | 5.8 | 134 |
| 30 | Enhancing Catalytic Activity of MoS<sub>2</sub> Basal Plane S-Vacancy by Co Cluster Addition. ACS Energy Letters, 2018, 3, 2685-2693. | 8.8 | 121 |
| 31 | Lightâ€Ðriven BiVO<sub>4</sub>â€“C Fuel Cell with Simultaneous Production of H<sub>2</sub>O<sub>2</sub>. Advanced Energy Materials, 2018, 8, 1801158. | 10.2 | 107 |
| 32 | Theoretical Investigations into Defected Graphene for Electrochemical Reduction of CO<sub>2</sub>. ACS Sustainable Chemistry and Engineering, 2017, 5, 11080-11085. | 3.2 | 93 |
| 33 | Introducing Fe<sup>2+</sup> into Nickelâ€“Iron Layered Double Hydroxide: Local Structure Modulated Water Oxidation Activity. Angewandte Chemie, 2018, 130, 9536-9540. | 1.6 | 86 |
| 34 | Precious Metal-Free Nickel Nitride Catalyst for the Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2019, 11, 26863-26871. | 4.0 | 81 |
| 35 | Theoretical Approaches to Describing the Oxygen Reduction Reaction Activity of Single-Atom Catalysts. Journal of Physical Chemistry C, 2018, 122, 29307-29318. | 1.5 | 68 |
| 36 | Influence of Adsorbed Water on the Oxygen Evolution Reaction on Oxides. Journal of Physical Chemistry C, 2015, 119, 1032-1037. | 1.5 | 66 |

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|---|---|---|---|
| 37 | High-performance oxygen reduction and evolution carbon catalysis: From mechanistic studies to device integration. Nano Research, 2017, 10, 1163-1177. | 5.8 | 66 |
| 38 | Orbital graph convolutional neural network for material property prediction. Physical Review Materials, 2020, 4, . | 0.9 | 64 |
| 39 | A review on electrocatalytic oxidation of methane to oxygenates. Journal of Materials Chemistry A, 2020, 8, 15575-15590. | 5.2 | 62 |
| 40 | Ligand-Engineered Metalâ€“Organic Frameworks for Electrochemical Reduction of Carbon Dioxide to Carbon Monoxide. ACS Catalysis, 2021, 11, 7350-7357. | 5.5 | 62 |
| 41 | Coproduction of hydrogen and lactic acid from glucose photocatalysis on band-engineered Zn1-xCdxS homojunction. IScience, 2021, 24, 102109. | 1.9 | 61 |
| 42 | Two-Dimensional Materials as Catalysts for Energy Conversion. Catalysis Letters, 2016, 146, 1917-1921. | 1.4 | 58 |
| 43 | Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene. ACS Central Science, 2017, 3, 1286-1293. | 5.3 | 54 |
| 44 | Tandem cathode for proton exchange membrane fuel cells. Physical Chemistry Chemical Physics, 2013, 15, 9326. | 1.3 | 53 |
| 45 | Catalytic hydrogenation of Cî€C and Cî€O in unsaturated fatty acid methyl esters. Catalysis Science and Technology, 2014, 4, 2427-2444. | 2.1 | 52 |
| 46 | Single Metal Atoms Anchored in Twoâ€Dimensional Materials: Bifunctional Catalysts for Fuel Cell Applications. ChemCatChem, 2018, 10, 3034-3039. | 1.8 | 50 |
| 47 | Ultrathin Cobalt Oxide Overlayer Promotes Catalytic Activity of Cobalt Nitride for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2018, 122, 4783-4791. | 1.5 | 46 |
| 48 | First principles investigation of zinc-anode dissolution in zincâ€“air batteries. Physical Chemistry Chemical Physics, 2013, 15, 6416. | 1.3 | 44 |
| 49 | Nature of Lone-Pairâ€“Surface Bonds and Their Scaling Relations. Inorganic Chemistry, 2018, 57, 7222-7238. | 1.9 | 43 |
| 50 | Improved Oxygen Reduction Reaction Activity of Nanostructured CoS<sub>2</sub> through Electrochemical Tuning. ACS Applied Energy Materials, 2019, 2, 8605-8614. | 2.5 | 42 |
| 51 | Copper Silver Thin Films with Metastable Miscibility for Oxygen Reduction Electrocatalysis in Alkaline Electrolytes. ACS Applied Energy Materials, 2018, 1, 1990-1999. | 2.5 | 40 |
| 52 | Structural and Energetic Trends of Ethylene Hydrogenation over Transition Metal Surfaces. Journal of Physical Chemistry C, 2016, 120, 995-1003. | 1.5 | 39 |
| 53 | H<sub>2</sub> production through electro-oxidation of SO<sub>2</sub>: identifying the fundamental limitations. Physical Chemistry Chemical Physics, 2014, 16, 9572-9579. | 1.3 | 36 |
| 54 | Circumventing Scaling Relations in Oxygen Electrochemistry Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2020, 11, 10029-10036. | 2.1 | 32 |

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|---|---|---|---|
| 55 | Rational design of carbon nitride for remarkable photocatalytic H2O2 production. Chem Catalysis, 2022, 2, 1720-1733. | 2.9 | 31 |
| 56 | 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. | 3.2 | 30 |
| 57 | Noble metal supported hexagonal boron nitride for the oxygen reduction reaction: a DFT study. Nanoscale Advances, 2019, 1, 132-139. | 2.2 | 29 |
| 58 | Highâ€Throughput Electron Diffraction Reveals a Hidden Novel Metalâ€“Organic Framework for Electrocatalysis. Angewandte Chemie - International Edition, 2021, 60, 11391-11397. | 7.2 | 29 |
| 59 | Ternary cobaltâ€“iron sulfide as a robust electrocatalyst for water oxidation: A dual effect from surface evolution and metal doping. Applied Surface Science, 2021, 542, 148681. | 3.1 | 28 |
| 60 | Electron affinity and redox potential of tetrafluoro-p-benzoquinone: A theoretical study. Journal of Fluorine Chemistry, 2008, 129, 222-225. | 0.9 | 24 |
| 61 | 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. | 4.0 | 24 |
| 62 | Development of Fukui Function Based Descriptors for a Machine Learning Study of CO2 Reduction. Journal of Physical Chemistry C, 2020, 124, 10079-10084. | 1.5 | 24 |
| 63 | Highâ€Performance Zincâ€Air Batteries Based on Bifunctional Hierarchically Porous Nitrogenâ€Doped Carbon. Small, 2022, 18, e2105928. | 5.2 | 23 |
| 64 | Calculation of two-electron reduction potentials for some quinone derivatives in aqueous solution using MÃ¸llerâ€“Plesset perturbation theory. Computational and Theoretical Chemistry, 2006, 759, 245-247. | 1.5 | 21 |
| 65 | Exploring Scaling Relations for Chemisorption Energies on Transitionâ€Metalâ€Exchanged Zeolites ZSMâ€22 and ZSMâ€5. ChemCatChem, 2016, 8, 767-772. | 1.8 | 18 |
| 66 | 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. | 1.5 | 16 |
| 67 | An insight into microscopic properties of aprotic ionic liquids: A DFT study. Computational and Theoretical Chemistry, 2010, 955, 47-52. | 1.5 | 16 |
| 68 | Elaborating Nitrogen and Oxygen Dopants Configurations within Graphene Electrocatalysts for Two-Electron Oxygen Reduction. , 2022, 4, 320-328. | | 15 |
| 69 | SnO<sub>2</sub>-supported single metal atoms: a bifunctional catalyst for the electrochemical synthesis of H<sub>2</sub>O<sub>2</sub>. Journal of Materials Chemistry A, 2022, 10, 6115-6121. | 5.2 | 14 |
| 70 | Activity and Selectivity for O<sub>2</sub> Reduction to H<sub>2</sub>O<sub>2</sub> on Transition Metal Surfaces. ECS Transactions, 2013, 58, 53-62. | 0.3 | 13 |
| 71 | Two-Dimensional Metalâ€“Organic Frameworks with Unique Oriented Layers for Oxygen Reduction Reaction: Tailoring the Activity through Exposed Crystal Facets. CCS Chemistry, 2022, 4, 1633-1642. | 4.6 | 13 |
| 72 | Trends in Adsorption Energies of the Oxygenated Species on Single Platinum Atom Embedded in Carbon Nanotubes. Catalysis Letters, 2017, 147, 2689-2696. | 1.4 | 10 |

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|---|---|---|---|
| 73 | Designing Carbon-Based Materials for Efficient Electrochemical Reduction of CO<sub>2</sub>. Industrial & Engineering Chemistry Research, 2019, 58, 879-885. | 1.8 | 10 |
| 74 | Effect of Adventitious Carbon on Pit Formation of Monolayer MoS 2. Advanced Materials, 2020, 32, 2003020. | 11.1 | 9 |
| 75 | Heteroatom-Doped Transition Metal Nitrides for CO Electrochemical Reduction: A Density Functional Theory Screening Study. Journal of Physical Chemistry C, 2020, 124, 26344-26351. | 1.5 | 8 |
| 76 | Exploring the Effect of Gold Support on the Oxygen Reduction Reaction Activity of Metal Porphycenes. ChemCatChem, 2018, 10, 5505-5510. | 1.8 | 6 |
| 77 | The role of Pt in Î±-MoC on the water-gas shift reaction at low temperatures. Joule, 2021, 5, 521-523. | 11.7 | 6 |
| 78 | Highâ€Throughput Electron Diffraction Reveals a Hidden Novel Metalâ€"Organic Framework for Electrocatalysis. Angewandte Chemie, 2021, 133, 11492-11498. | 1.6 | 6 |
| 79 | Effect of doping TiO<sub>2</sub> with Mn for electrocatalytic oxidation in acid and alkaline electrolytes. Energy Advances, 2022, 1, 357-366. | 1.4 | 4 |
| 80 | Enhancing Oxygen Reduction Reaction Activity Using Single Atom Catalyst Supported on Tantalum Pentoxide. ChemCatChem, 0, , . | 1.8 | 1 |
| 81 | Pit Formation Mechanism of Monolayer MoS2 By Thermal Oxidation. ECS Meeting Abstracts, 2020, MA2020-02, 3887-3887. | 0.0 | 0 |
| 82 | Cuâ€doped Ba<sub>0.5</sub>Sr<sub>0.5</sub>FeO<sub>3â€Î´</sub> for electrochemical synthesis of hydrogen peroxide via a 2â€electron oxygen reduction reaction<sup>1</sup>. Electrochemical Science Advances, 2023, 3, . | 1.2 | 0 |