

Maytal Caspary Toroker

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

86
papers

2,025
citations

21
h-index

42
g-index

96
ext. papers

2,402
ext. citations

6.8
avg, IF

5.64
L-index

#	Paper	IF	Citations
86	First principles scheme to evaluate band edge positions in potential transition metal oxide photocatalysts and photoelectrodes. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 16644-54	3.6	287
85	Electron transport in pure and doped hematite. <i>Nano Letters</i> , 2011 , 11, 1775-81	11.5	227
84	Operando X-Ray Absorption Spectroscopy Shows Iron Oxidation Is Concurrent with Oxygen Evolution in Cobalt-Iron (Oxy)hydroxide Electrocatalysts. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 12840-12844	16.4	90
83	Ternary Ni-Co-Fe oxyhydroxide oxygen evolution catalysts: Intrinsic activity trends, electrical conductivity, and electronic band structure. <i>Nano Research</i> , 2019 , 12, 2288-2295	10	76
82	Influence of Electrolyte Cations on Ni(Fe)OOH Catalyzed Oxygen Evolution Reaction. <i>Chemistry of Materials</i> , 2017 , 29, 4761-4767	9.6	74
81	Toward Settling the Debate on the Role of Fe ₂ O ₃ Surface States for Water Splitting. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 24789-24795	3.8	73
80	The "Rust" Challenge: On the Correlations between Electronic Structure, Excited State Dynamics, and Photoelectrochemical Performance of Hematite Photoanodes for Solar Water Splitting. <i>Advanced Materials</i> , 2018 , 30, e1706577	24	69
79	Platinum-Doped Fe ₂ O ₃ for Enhanced Water Splitting Efficiency: A DFT+U Study. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 5836-5847	3.8	64
78	Transition metal oxide alloys as potential solar energy conversion materials. <i>Journal of Materials Chemistry A</i> , 2013 , 1, 2474	13	55
77	Hydrogen Oxidation on Ni-Based Electrocatalysts: The Effect of Metal Doping. <i>Catalysts</i> , 2018 , 8, 454	4	55
76	Theoretical Insights into the Mechanism of Water Oxidation on Nonstoichiometric and Titanium-Doped Fe ₂ O ₃ (0001). <i>Journal of Physical Chemistry C</i> , 2014 , 118, 23162-23167	3.8	47
75	A First-Principles Study on the Role of an Al ₂ O ₃ Overlayer on Fe ₂ O ₃ for Water Splitting. <i>ACS Catalysis</i> , 2015 , 5, 7237-7243	13.1	47
74	Significant reduction in NiO band gap upon formation of Li _x Ni _{1-x} O alloys: applications to solar energy conversion. <i>ChemSusChem</i> , 2014 , 7, 195-201	8.3	45
73	The secret behind the success of doping nickel oxyhydroxide with iron. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 7491-7497	3.6	38
72	Electronic transport through molecular junctions with nonrigid molecule-leads coupling. <i>Journal of Chemical Physics</i> , 2007 , 127, 154706	3.9	37
71	Enhanced Water Oxidation Catalysis of Nickel Oxyhydroxide through the Addition of Vacancies. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 25405-25410	3.8	36
70	Benchmarking Density Functional Theory Based Methods To Model NiOOH Material Properties: Hubbard and van der Waals Corrections vs Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3807-12	6.4	33

69	Revisiting photoemission and inverse photoemission spectra of nickel oxide from first principles: implications for solar energy conversion. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 7963-71	3.4	32
68	Engineering Band Edge Positions of Nickel Oxyhydroxide through Facet Selection. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 8104-8108	3.8	27
67	Water Oxidation Catalysis with Fe ₂ O ₃ Constrained at the Nanoscale. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 6120-6125	3.8	24
66	Can we judge an oxide by its cover? The case of platinum over Fe ₂ O ₃ from first principles. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 24129-37	3.6	21
65	Understanding the Oxygen Evolution Reaction on a Two-Dimensional NiO ₂ Catalyst. <i>ChemElectroChem</i> , 2017 , 4, 2764-2770	4.3	21
64	Three fundamental questions on one of our best water oxidation catalysts: a critical perspective. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	20
63	Hazardous Doping for Photo-Electrochemical Conversion: The Case of Nb-Doped Fe ₂ O ₃ from First Principles. <i>Molecules</i> , 2015 , 20, 19900-6	4.8	20
62	Play the heavy: An effective mass study for Fe ₂ O ₃ and corundum oxides. <i>Journal of Chemical Physics</i> , 2016 , 144, 164704	3.9	20
61	Identifying the bottleneck of water oxidation by ab initio analysis of in situ optical absorbance spectrum. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 17278-17286	3.6	19
60	Hole Transport in Nonstoichiometric and Doped W ₂ O ₆ . <i>Journal of Physical Chemistry C</i> , 2012 , 116, 17403-17413	3.7	18
59	Site-directed electronic tunneling in a dissipative molecular environment. <i>Journal of Chemical Physics</i> , 2008 , 129, 034501	3.9	18
58	Designing efficient doped NiOOH catalysts for water splitting with first principles calculations. <i>ChemistrySelect</i> , 2016 , 1, 911-916	1.8	18
57	CVD-grown copper tungstate thin films for solar water splitting. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 10206-10216	13	17
56	Metal-Oxygen Bond Ionicity as an Efficient Descriptor for Doped NiOOH Photocatalytic Activity. <i>ChemPhysChem</i> , 2016 , 17, 1630-6	3.2	17
55	Ternary NiFeTiOOH Catalyst for the Oxygen Evolution Reaction: Study of the Effect of the Addition of Ti at Different Loadings. <i>ACS Catalysis</i> , 2020 , 10, 4879-4887	13.1	15
54	Controlled electronic transport through branched molecular conductors. <i>Molecular Physics</i> , 2008 , 106, 281-287	1.7	15
53	Mn Cations Control Electronic Transport in Spinel Co _x Mn _{3-x} O ₄ Nanoparticles. <i>Chemistry of Materials</i> , 2019 , 31, 4228-4233	9.6	14
52	Strong Band Gap Blueshift in Copper (I) Oxide Semiconductor via Bioinspired Route. <i>Advanced Functional Materials</i> , 2020 , 30, 1910405	15.6	14

51	Electronic Properties of Pure and Fe-Doped Ni(OH)_2 : New Insights Using Density Functional Theory with a Cluster Approach. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 12344-12350	3.8	14
50	Dual Mechanisms: Hydrogen Transfer during Water Oxidation Catalysis of Pure and Fe-Doped Nickel Oxyhydroxide. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 16819-16824	3.8	14
49	Lateral Chemical Bonding in Two-Dimensional Transition-Metal Dichalcogenide Metal/Semiconductor Heterostructures. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 5401-5410	3.8	13
48	Manipulating electrochemical performance through doping beyond the solubility limit. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 16098-105	3.6	13
47	Modeling Diffusion in Functional Materials: From Density Functional Theory to Artificial Intelligence. <i>Advanced Functional Materials</i> , 2020 , 30, 1900778	15.6	13
46	Communication: Nickel hydroxide as an exceptional deviation from the quantum size effect. <i>Journal of Chemical Physics</i> , 2018 , 149, 141103	3.9	13
45	Operando X-Ray Absorption Spectroscopy Shows Iron Oxidation Is Concurrent with Oxygen Evolution in Cobalt/Iron (Oxy)hydroxide Electrocatalysts. <i>Angewandte Chemie</i> , 2018 , 130, 13022-13026	3.6	13
44	Novel High-Throughput Screening Approach for Functional Metal/Oxide Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1572-82	6.4	12
43	Electronic Structure of Catalysis Intermediates by the G0W0 Approximation. <i>Catalysis Letters</i> , 2016 , 146, 2009-2014	2.8	12
42	Nickel phosphide decorated with trace amount of platinum as an efficient electrocatalyst for the alkaline hydrogen evolution reaction. <i>Sustainable Energy and Fuels</i> , 2019 , 3, 2006-2014	5.8	11
41	Water Oxidation Catalysis for NiOOH by a Metropolis Monte Carlo Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2380-2385	6.4	11
40	Selective ligand removal to improve accessibility of active sites in hierarchical MOFs for heterogeneous photocatalysis. <i>Nature Communications</i> , 2022 , 13, 282	17.4	11
39	Theoretical Investigation of Dielectric Materials for Two-Dimensional Field-Effect Transistors. <i>Advanced Functional Materials</i> , 2020 , 30, 1808544	15.6	11
38	Site-directed deep electronic tunneling through a molecular network. <i>Journal of Chemical Physics</i> , 2005 , 123, 151101	3.9	10
37	Optimization of Ni-Co-Fe-Based Catalysts for Oxygen Evolution Reaction by Surface and Relaxation Phenomena Analysis. <i>ChemSusChem</i> , 2021 , 14, 1737-1746	8.3	10
36	Progress in understanding hematite electrochemistry through computational modeling. <i>Computational Materials Science</i> , 2019 , 160, 411-419	3.2	8
35	Strategies to suppress cation vacancies in metal oxide alloys: consequences for solar energy conversion. <i>Journal of Materials Science</i> , 2015 , 50, 5715-5722	4.3	8
34	On the effect of nuclear bridge modes on donor-acceptor electronic coupling in donor-bridge-acceptor molecules. <i>Chemical Physics</i> , 2009 , 358, 45-51	2.3	8

33	The Effect of Covering Fe ₂ O ₃ with a Ga ₂ O ₃ Overlayer on Water Oxidation Catalysis. <i>Catalysis Letters</i> , 2017 , 147, 2077-2082	2.8	8
32	The Operando Optical Spectrum of Hematite during Water Splitting through a -BSE Calculation. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 4857-4864	6.4	7
31	Unveiling ionic diffusion in MgNiMnO ₄ cathode material for Mg-ion batteries via combined computational and experimental studies. <i>Journal of Solid State Electrochemistry</i> , 2019 , 23, 3209-3216	2.6	7
30	Thermal rate constants for resonance-supporting reaction barriers by the flux averaging method. <i>Chemical Physics Letters</i> , 2003 , 369, 232-239	2.5	7
29	On the nature of trapped states in an MoS ₂ two-dimensional semiconductor with sulfur vacancies. <i>Molecular Physics</i> , 2019 , 117, 2058-2068	1.7	7
28	Efficient cationic agents for exfoliating two-dimensional nickel oxide sheets. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	6
27	Metallic back-contact interface design in photoelectrochemical devices. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 8989-8996	7.1	6
26	Bifunctional PGM-free metal organic framework-based electrocatalysts for alkaline electrolyzers: trends in the activity with different metal centers. <i>Nanoscale</i> , 2021 , 13, 4576-4584	7.7	6
25	Materials with honeycomb structures for gate dielectrics in two-dimensional Field Effect Transistors [An ab initio study. <i>Ceramics International</i> , 2019 , 45, 9339-9347	5.1	5
24	A quantum mechanical flux correlation approach to steady-state transport rates in molecular junctions. <i>Chemical Physics</i> , 2010 , 370, 124-131	2.3	5
23	Site-directed electronic tunneling through a vibrating molecular network. <i>Journal of Chemical Physics</i> , 2006 , 125, 184703	3.9	5
22	Breakdown of the Small-Polaron Hopping Model in Higher-Order Spinel. <i>Advanced Materials</i> , 2020 , 32, e2004490	24	5
21	Dipole-Induced Raman Enhancement Using Noncovalent Azobenzene-Functionalized Self-Assembled Monolayers on Graphene Terraces. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 10271-10278	9.5	5
20	The electronic structure of two-dimensional transition metal hydroxide monolayers and heterostructures. <i>Solid State Ionics</i> , 2018 , 314, 149-155	3.3	5
19	Challenges of modeling nanostructured materials for photocatalytic water splitting.. <i>Chemical Society Reviews</i> , 2022 ,	58.5	5
18	Hydrogen transfer through different crystal phases of nickel oxy/hydroxide. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25169-25178	3.6	4
17	Revealing the Conducting Character of the NiOOH Catalyst through Defect Chemistry. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 18895-18904	3.8	4
16	Electronic structure of NiOOH with hydrogen vacancies and implications for energy conversion applications. <i>MRS Communications</i> , 2017 , 7, 206-213	2.7	3

15	Optimal Oxygen Vacancy Concentration for CO ₂ Reduction in LSFCr Perovskite: A Combined Density Functional Theory and Thermogravimetric Analysis Measurement Study. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 27453-27466	3.8	3
14	Toward Ambitious Multiscale Modeling of Nanocrystal Catalysts for Water Splitting. <i>ACS Energy Letters</i> , 2020 , 5, 2042-2044	20.1	2
13	The Effect of Fe and Co Additions on the Efficiency of NiOOH Catalyst Under Strain. <i>ChemCatChem</i> , 2020 , 12, 2801-2806	5.2	2
12	Practical Cluster Models for a Layered NiOOH Material. <i>Materials</i> , 2017 , 10,	3.5	2
11	Thermal resonant tunneling rates by a generalized flux averaging method. <i>Israel Journal of Chemistry</i> , 2002 , 42, 237-244	3.4	2
10	A comparative study of Bi, Sb, and BiSb for electrochemical nitrogen reduction leading to a new catalyst design strategy. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 20453-20465	13	2
9	Enhanced Li-ion diffusion and electrochemical performance in strained-manganese-iron oxide core-shell nanoparticles. <i>Journal of Chemical Physics</i> , 2021 , 155, 144702	3.9	1
8	Charge Transport Calculation along Two-Dimensional Metal/Semiconductor/Metal Systems. <i>Israel Journal of Chemistry</i> , 2020 , 60, 888-896	3.4	1
7	Pathways for charge transport through material interfaces. <i>Journal of Chemical Physics</i> , 2020 , 153, 024104	3.9	0
6	Perovskite La _{0.3} Sr _{0.7} Fe _{0.7} Cr _{0.3} O ₃ Catalysis Raises the Bar: Preventing Unwanted Near-Surface Sr Segregation and SrCO ₃ Precipitation. <i>Advanced Theory and Simulations</i> , 2100173	3.5	0
5	Changing your tune on catalytic efficiency: Tuning Cr concentration in La _{0.3} Sr _{0.7} Fe _{1-x} Cr _x O ₃ -□ perovskite as a cathode in solid oxide electrolysis cell. <i>Computational Materials Science</i> , 2022 , 210, 111462	3.2	0
4	Electronic Charge Transport: Breakdown of the Small-Polaron Hopping Model in Higher-Order Spinel (Adv. Mater. 49/2020). <i>Advanced Materials</i> , 2020 , 32, 2070368	24	
3	Simultaneous propagation of different wavepackets driven by lasers. <i>Chemical Physics Letters</i> , 2006 , 431, 169-173	2.5	
2	Strain Controlling Catalytic Efficiency of Water Oxidation for Ni _{1-x} Fe _x OOH Alloy. <i>Molecular Modeling and Simulation</i> , 2021 , 1-23		
1	Explanation of the Opposing Shifts in the Absorption Edge and the Optical Resonance in CuFeS ₂ Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 5592-5597	3.8	