Maytal Caspary Toroker

List of Publications by Year in Descending Order

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	Selective ligand removal to improve accessibility of active sites in hierarchical MOFs for heterogeneous photocatalysis.. *Nature Communications*, **2022**, 13, 282	17.4	11
85	Explanation of the Opposing Shifts in the Absorption Edge and the Optical Resonance in CuFeS2 Nanoparticles. *Journal of Physical Chemistry C*, **2022**, 126, 5592-5597	3.8	
84	Challenges of modeling nanostructured materials for photocatalytic water splitting.. *Chemical Society Reviews*, **2022**,	58.5	5
83	Changing your tune on catalytic efficiency: Tuning Cr concentration in La0.3Sr0.7Fe1-xCrxO3- perovskite as a cathode in solid oxide electrolysis cell. *Computational Materials Science*, **2022**, 210, 111462	3.2	0
82	Enhanced Li-ion diffusion and electrochemical performance in strained-manganese-iron oxide core-shell nanoparticles. *Journal of Chemical Physics*, **2021**, 155, 144702	3.9	1
81	Bifunctional PGM-free metal organic framework-based electrocatalysts for alkaline electrolyzers: trends in the activity with different metal centers. *Nanoscale*, **2021**, 13, 4576-4584	7.7	6
80	A comparative study of Bi, Sb, and BiSb for electrochemical nitrogen reduction leading to a new catalyst design strategy. *Journal of Materials Chemistry A*, **2021**, 9, 20453-20465	13	2
79	Optimization of Ni-Co-Fe-Based Catalysts for Oxygen Evolution Reaction by Surface and Relaxation Phenomena Analysis. *ChemSusChem*, **2021**, 14, 1737-1746	8.3	10
78	Dipole-Induced Raman Enhancement Using Noncovalent Azobenzene-Functionalized Self-Assembled Monolayers on Graphene Terraces. *ACS Applied Materials & Interfaces*, **2021**, 13, 10271-10278	9.5	5
77	Strain Controlling Catalytic Efficiency of Water Oxidation for Ni1FexOOH Alloy. *Molecular Modeling and Simulation*, **2021**, 1-23		
76	Electronic Charge Transport: Breakdown of the Small-Polaron Hopping Model in Higher-Order Spinels (Adv. Mater. 49/2020). *Advanced Materials*, **2020**, 32, 2070368	24	
75	Toward Ambitious Multiscale Modeling of Nanocrystal Catalysts for Water Splitting. *ACS Energy Letters*, **2020**, 5, 2042-2044	20.1	2
74	The Effect of Fe and Co Additions on the Efficiency of NiOOH Catalyst Under Strain. *ChemCatChem*, **2020**, 12, 2801-2806	5.2	2
73	Ternary NiFeTiOOH Catalyst for the Oxygen Evolution Reaction: Study of the Effect of the Addition of Ti at Different Loadings. *ACS Catalysis*, **2020**, 10, 4879-4887	13.1	15
72	The Operando Optical Spectrum of Hematite during Water Splitting through a -BSE Calculation. *Journal of Chemical Theory and Computation*, **2020**, 16, 4857-4864	6.4	7
71	Strong Band Gap Blueshift in Copper (I) Oxide Semiconductor via Bioinspired Route. *Advanced Functional Materials*, **2020**, 30, 1910405	15.6	14
70	Charge Transport Calculation along Two-Dimensional Metal/Semiconductor/Metal Systems. *Israel Journal of Chemistry*, **2020**, 60, 888-896	3.4	1

69	Breakdown of the Small-Polaron Hopping Model in Higher-Order Spinels. *Advanced Materials*, **2020**, 32, e2004490	24	5
68	Optimal Oxygen Vacancy Concentration for CO2 Reduction in LSFCr Perovskite: A Combined Density Functional Theory and Thermogravimetric Analysis Measurement Study. *Journal of Physical Chemistry C*, **2020**, 124, 27453-27466	3.8	3
67	Pathways for charge transport through material interfaces. *Journal of Chemical Physics*, **2020**, 153, 024104	3.9	0
66	Theoretical Investigation of Dielectric Materials for Two-Dimensional Field-Effect Transistors. *Advanced Functional Materials*, **2020**, 30, 1808544	15.6	11
65	Modeling Diffusion in Functional Materials: From Density Functional Theory to Artificial Intelligence. *Advanced Functional Materials*, **2020**, 30, 1900778	15.6	13
64	Progress in understanding hematite electrochemistry through computational modeling. *Computational Materials Science*, **2019**, 160, 411-419	3.2	8
63	Nickel phosphide decorated with trace amount of platinum as an efficient electrocatalyst for the alkaline hydrogen evolution reaction. *Sustainable Energy and Fuels*, **2019**, 3, 2006-2014	5.8	11
62	Mn Cations Control Electronic Transport in Spinel CoxMn3□O4 Nanoparticles. *Chemistry of Materials*, **2019**, 31, 4228-4233	9.6	14
61	Ternary Ni-Co-Fe oxyhydroxide oxygen evolution catalysts: Intrinsic activity trends, electrical conductivity, and electronic band structure. *Nano Research*, **2019**, 12, 2288-2295	10	76
60	Materials with honeycomb structures for gate dielectrics in two-dimensional Field Effect Transistors □An ab initio study. *Ceramics International*, **2019**, 45, 9339-9347	5.1	5
59	Revealing the Conducting Character of the □NiOOH Catalyst through Defect Chemistry. *Journal of Physical Chemistry C*, **2019**, 123, 18895-18904	3.8	4
58	Unveiling ionic diffusion in MgNiMnO4 cathode material for Mg-ion batteries via combined computational and experimental studies. *Journal of Solid State Electrochemistry*, **2019**, 23, 3209-3216	2.6	7
57	On the nature of trapped states in an MoS2 two-dimensional semiconductor with sulfur vacancies. *Molecular Physics*, **2019**, 117, 2058-2068	1.7	7
56	The "Rust" Challenge: On the Correlations between Electronic Structure, Excited State Dynamics, and Photoelectrochemical Performance of Hematite Photoanodes for Solar Water Splitting. *Advanced Materials*, **2018**, 30, e1706577	24	69
55	CVD-grown copper tungstate thin films for solar water splitting. *Journal of Materials Chemistry A*, **2018**, 6, 10206-10216	13	17
54	Water Oxidation Catalysis for NiOOH by a Metropolis Monte Carlo Algorithm. *Journal of Chemical Theory and Computation*, **2018**, 14, 2380-2385	6.4	11
53	Lateral Chemical Bonding in Two-Dimensional Transition-Metal Dichalcogenide Metal/Semiconductor Heterostructures. *Journal of Physical Chemistry C*, **2018**, 122, 5401-5410	3.8	13
52	Efficient cationic agents for exfoliating two-dimensional nickel oxide sheets. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	6

51	Operando X-Ray Absorption Spectroscopy Shows Iron Oxidation Is Concurrent with Oxygen Evolution in Cobalt-Iron (Oxy)hydroxide Electrocatalysts. *Angewandte Chemie - International Edition* , **2018**, 57, 12840-12844	16.4	90
50	Hydrogen transfer through different crystal phases of nickel oxy/hydroxide. *Physical Chemistry Chemical Physics*, **2018**, 20, 25169-25178	3.6	4
49	The electronic structure of two-dimensional transition metal hydroxide monolayers and heterostructures. *Solid State Ionics*, **2018**, 314, 149-155	3.3	5
48	Communication: Nickel hydroxide as an exceptional deviation from the quantum size effect. *Journal of Chemical Physics*, **2018**, 149, 141103	3.9	13
47	Hydrogen Oxidation on Ni-Based Electrocatalysts: The Effect of Metal Doping. *Catalysts*, **2018**, 8, 454	4	55
46	Operando X-Ray Absorption Spectroscopy Shows Iron Oxidation Is Concurrent with Oxygen Evolution in Cobalt□Iron (Oxy)hydroxide Electrocatalysts. *Angewandte Chemie*, **2018**, 130, 13022-13026	3.6	13
45	Water Oxidation Catalysis with Fe2O3 Constrained at the Nanoscale. *Journal of Physical Chemistry C* , **2017**, 121, 6120-6125	3.8	24
44	The secret behind the success of doping nickel oxyhydroxide with iron. *Physical Chemistry Chemical Physics*, **2017**, 19, 7491-7497	3.6	38
43	Electronic structure of □NiOOH with hydrogen vacancies and implications for energy conversion applications. *MRS Communications*, **2017**, 7, 206-213	2.7	3
42	Influence of Electrolyte Cations on Ni(Fe)OOH Catalyzed Oxygen Evolution Reaction. *Chemistry of Materials*, **2017**, 29, 4761-4767	9.6	74
41	Identifying the bottleneck of water oxidation by ab initio analysis of in situ optical absorbance spectrum. *Physical Chemistry Chemical Physics*, **2017**, 19, 17278-17286	3.6	19
40	Understanding the Oxygen Evolution Reaction on a Two-Dimensional NiO2 Catalyst. *ChemElectroChem*, **2017**, 4, 2764-2770	4.3	21
39	Dual Mechanisms: Hydrogen Transfer during Water Oxidation Catalysis of Pure and Fe-Doped Nickel Oxyhydroxide. *Journal of Physical Chemistry C*, **2017**, 121, 16819-16824	3.8	14
38	Practical Cluster Models for a Layered □NiOOH Material. *Materials*, **2017**, 10,	3.5	2
37	The Effect of Covering Fe2O3 with a Ga2O3 Overlayer on Water Oxidation Catalysis. *Catalysis Letters*, **2017**, 147, 2077-2082	2.8	8
36	Benchmarking Density Functional Theory Based Methods To Model NiOOH Material Properties: Hubbard and van der Waals Corrections vs Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2016**, 12, 3807-12	6.4	33
35	Enhanced Water Oxidation Catalysis of Nickel Oxyhydroxide through the Addition of Vacancies. *Journal of Physical Chemistry C*, **2016**, 120, 25405-25410	3.8	36
34	Three fundamental questions on one of our best water oxidation catalysts: a critical perspective. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	20

33	Electronic Properties of Pure and Fe-Doped Ni(OH)2: New Insights Using Density Functional Theory with a Cluster Approach. *Journal of Physical Chemistry C*, **2016**, 120, 12344-12350	3.8	14
32	Metal-Oxygen Bond Ionicity as an Efficient Descriptor for Doped NiOOH Photocatalytic Activity. *ChemPhysChem*, **2016**, 17, 1630-6	3.2	17
31	Play the heavy: An effective mass study for Fe2O3 and corundum oxides. *Journal of Chemical Physics*, **2016**, 144, 164704	3.9	20
30	Novel High-Throughput Screening Approach for Functional Metal/Oxide Interfaces. *Journal of Chemical Theory and Computation*, **2016**, 12, 1572-82	6.4	12
29	Engineering Band Edge Positions of Nickel Oxyhydroxide through Facet Selection. *Journal of Physical Chemistry C*, **2016**, 120, 8104-8108	3.8	27
28	Metallic back-contact interface design in photoelectrochemical devices. *Journal of Materials Chemistry C*, **2016**, 4, 8989-8996	7.1	6
27	Manipulating electrochemical performance through doping beyond the solubility limit. *Physical Chemistry Chemical Physics*, **2016**, 18, 16098-105	3.6	13
26	Electronic Structure of Catalysis Intermediates by the G0W0 Approximation. *Catalysis Letters*, **2016**, 146, 2009-2014	2.8	12
25	Designing efficient doped NiOOH catalysts for water splitting with first principles calculations. *ChemistrySelect*, **2016**, 1, 911-916	1.8	18
24	Toward Settling the Debate on the Role of Fe2O3 Surface States for Water Splitting. *Journal of Physical Chemistry C*, **2015**, 119, 24789-24795	3.8	73
23	Can we judge an oxide by its cover? The case of platinum over Fe2O3 from first principles. *Physical Chemistry Chemical Physics*, **2015**, 17, 24129-37	3.6	21
22	Hazardous Doping for Photo-Electrochemical Conversion: The Case of Nb-Doped Fe from First Principles. *Molecules*, **2015**, 20, 19900-6	4.8	20
21	Platinum-Doped Fe2O3 for Enhanced Water Splitting Efficiency: A DFT+U Study. *Journal of Physical Chemistry C*, **2015**, 119, 5836-5847	3.8	64
20	Strategies to suppress cation vacancies in metal oxide alloys: consequences for solar energy conversion. *Journal of Materials Science*, **2015**, 50, 5715-5722	4.3	8
19	A First-Principles Study on the Role of an Al2O3 Overlayer on Fe2O3 for Water Splitting. *ACS Catalysis*, **2015**, 5, 7237-7243	13.1	47
18	Revisiting photoemission and inverse photoemission spectra of nickel oxide from first principles: implications for solar energy conversion. *Journal of Physical Chemistry B*, **2014**, 118, 7963-71	3.4	32
17	Theoretical Insights into the Mechanism of Water Oxidation on Nonstoichiometric and Titanium-Doped Fe2O3(0001). *Journal of Physical Chemistry C*, **2014**, 118, 23162-23167	3.8	47
16	Significant reduction in NiO band gap upon formation of Lix Ni1-x O alloys: applications to solar energy conversion. *ChemSusChem*, **2014**, 7, 195-201	8.3	45

15	Transition metal oxide alloys as potential solar energy conversion materials. *Journal of Materials Chemistry A*, **2013**, 1, 2474	13	55
14	Hole Transport in Nonstoichiometric and Doped W□tite. *Journal of Physical Chemistry C*, **2012**, 116, 17403-17413	3.8	38
13	First principles scheme to evaluate band edge positions in potential transition metal oxide photocatalysts and photoelectrodes. *Physical Chemistry Chemical Physics*, **2011**, 13, 16644-54	3.6	287
12	Electron transport in pure and doped hematite. *Nano Letters*, **2011**, 11, 1775-81	11.5	227
11	A quantum mechanical flux correlation approach to steady-state transport rates in molecular junctions. *Chemical Physics*, **2010**, 370, 124-131	2.3	5
10	On the effect of nuclear bridge modes on donor□cceptor electronic coupling in donor□ridge□cceptor molecules. *Chemical Physics*, **2009**, 358, 45-51	2.3	8
9	Site-directed electronic tunneling in a dissipative molecular environment. *Journal of Chemical Physics*, **2008**, 129, 034501	3.9	18
8	Controlled electronic transport through branched molecular conductors. *Molecular Physics*, **2008**, 106, 281-287	1.7	15
7	Electronic transport through molecular junctions with nonrigid molecule-leads coupling. *Journal of Chemical Physics*, **2007**, 127, 154706	3.9	37
6	Site-directed electronic tunneling through a vibrating molecular network. *Journal of Chemical Physics*, **2006**, 125, 184703	3.9	5
5	Simultaneous propagation of different wavepackets driven by lasers. *Chemical Physics Letters*, **2006** , 431, 169-173	2.5	
4	Site-directed deep electronic tunneling through a molecular network. *Journal of Chemical Physics*, **2005**, 123, 151101	3.9	10
3	Thermal rate constants for resonance-supporting reaction barriers by the flux averaging method. *Chemical Physics Letters*, **2003**, 369, 232-239	2.5	7
2	Thermal resonant tunneling rates by a generalized flux averaging method. *Israel Journal of Chemistry*, **2002**, 42, 237-244	3.4	2
1	Perovskite La0.3Sr0.7Fe0.7Cr0.3O3□Catalysis Raises the Bar: Preventing Unwanted Near-Surface Sr Segregation and SrCO3 Precipitation. *Advanced Theory and Simulations*,2100173	3.5	0