Maytal Caspary Toroker

List of Publications by Year
in descending order

95 papers	2,856 citations	218381 26 h-index	189595 50 g-index
96 all docs	96 docs citations	96 times ranked	3813 citing authors

#	Article	IF	Citations
1	First principles scheme to evaluate band edge positions in potential transition metal oxide photocatalysts and photoelectrodes. Physical Chemistry Chemical Physics, 2011, 13, 16644.	1.3	380
2	Electron Transport in Pure and Doped Hematite. Nano Letters, 2011, 11, 1775-1781.	4.5	267
3	Ternary Ni-Co-Fe oxyhydroxide oxygen evolution catalysts: Intrinsic activity trends, electrical conductivity, and electronic band structure. Nano Research, 2019, 12, 2288-2295.	5.8	134
4	Operando Xâ€Ray Absorption Spectroscopy Shows Iron Oxidation Is Concurrent with Oxygen Evolution in Cobaltâ€“Iron (Oxy)hydroxide Electrocatalysts. Angewandte Chemie - International Edition, 2018, 57, 12840-12844.	7.2	131
5	Influence of Electrolyte Cations on Ni(Fe)OOH Catalyzed Oxygen Evolution Reaction. Chemistry of Materials, 2017, 29, 4761-4767.	3.2	105
6	Toward Settling the Debate on the Role of Fe₂O₃ Surface States for Water Splitting. Journal of Physical Chemistry C, 2015, 119, 24789-24795.	1.5	87
7	The â€œRustâ€•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.	11.1	83
8	Selective ligand removal to improve accessibility of active sites in hierarchical MOFs for heterogeneous photocatalysis. Nature Communications, 2022, 13, 282.	5.8	83
9	Hydrogen Oxidation on Ni-Based Electrocatalysts: The Effect of Metal Doping. Catalysts, 2018, 8, 454.	1.6	80
10	Platinum-Doped Î±-Fe₂O₃for Enhanced Water Splitting Efficiency: A DFT+UStudy. Journal of Physical Chemistry C, 2015, 119, 5836-5847.	1.5	73
11	Challenges of modeling nanostructured materials for photocatalytic water splitting. Chemical Society Reviews, 2022, 51, 3794-3818.	18.7	64
12	Transition metal oxide alloys as potential solar energy conversion materials. Journal of Materials Chemistry A, 2013, 1, 2474.	5.2	63
13	Significant Reduction in NiO Band Gap Upon Formation of Li_xNi_{1â^'x}O alloys: Applications To Solar Energy Conversion. ChemSusChem, 2014, 7, 195-201.	3.6	56
14	Theoretical Insights into the Mechanism of Water Oxidation on Nonstoichiometric and Titanium-Doped Fe₂O₃(0001). Journal of Physical Chemistry C, 2014, 118, 23162-23167.	1.5	52
15	The secret behind the success of doping nickel oxyhydroxide with iron. Physical Chemistry Chemical Physics, 2017, 19, 7491-7497.	1.3	51
16	A First-Principles Study on the Role of an Al₂O₃ Overlayer on Fe₂O₃ for Water Splitting. ACS Catalysis, 2015, 5, 7237-7243.	5.5	50
17	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, 3807-3812.	2.3	47
18	Enhanced Water Oxidation Catalysis of Nickel Oxyhydroxide through the Addition of Vacancies. Journal of Physical Chemistry C, 2016, 120, 25405-25410.	1.5	43

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19	Electronic transport through molecular junctions with nonrigid molecule-leads coupling. Journal of Chemical Physics, 2007, 127, 154706.	1.2	40
20	Revisiting Photoemission and Inverse Photoemission Spectra of Nickel Oxide from First Principles: Implications for Solar Energy Conversion. Journal of Physical Chemistry B, 2014, 118, 7963-7971.	1.2	39
21	Engineering Band Edge Positions of Nickel Oxyhydroxide through Facet Selection. Journal of Physical Chemistry C, 2016, 120, 8104-8108.	1.5	34
22	Modeling Diffusion in Functional Materials: From Density Functional Theory to Artificial Intelligence. Advanced Functional Materials, 2020, 30, 1900778.	7.8	33
23	Understanding the Oxygen Evolution Reaction on a Twoâ€Dimensional NiO₂ Catalyst. ChemElectroChem, 2017, 4, 2764-2770.	1.7	29
24	Play the heavy: An effective mass study for Î±-Fe2O3 and corundum oxides. Journal of Chemical Physics, 2016, 144, 164704.	1.2	28
25	Water Oxidation Catalysis with Fe₂O₃ Constrained at the Nanoscale. Journal of Physical Chemistry C, 2017, 121, 6120-6125.	1.5	28
26	Operando Xâ€Ray Absorption Spectroscopy Shows Iron Oxidation Is Concurrent with Oxygen Evolution in Cobaltâ€“Iron (Oxy)hydroxide Electrocatalysts. Angewandte Chemie, 2018, 130, 13022-13026.	1.6	28
27	Hazardous Doping for Photo-Electrochemical Conversion: The Case of Nb-Doped Fe2O3 from First Principles. Molecules, 2015, 20, 19900-19906.	1.7	27
28	Designing efficient doped NiOOH catalysts for water splitting with first principles calculations. ChemistrySelect, 2016, 1, 911-916.	0.7	26
29	Mn Cations Control Electronic Transport in Spinel Co_xMn_{3â€“x}O₄ Nanoparticles. Chemistry of Materials, 2019, 31, 4228-4233.	3.2	26
30	Metalâ€“Oxygen Bond Ionicity as an Efficient Descriptor for Doped NiOOH Photocatalytic Activity. ChemPhysChem, 2016, 17, 1630-1636.	1.0	25
31	Three fundamental questions on one of our best water oxidation catalysts: a critical perspective. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
32	Identifying the bottleneck of water oxidation by ab initio analysis of in situ optical absorbance spectrum. Physical Chemistry Chemical Physics, 2017, 19, 17278-17286.	1.3	25
33	CVD-grown copper tungstate thin films for solar water splitting. Journal of Materials Chemistry A, 2018, 6, 10206-10216.	5.2	25
34	Can we judge an oxide by its cover? The case of platinum over Î±-Fe₂O₃ from first principles. Physical Chemistry Chemical Physics, 2015, 17, 24129-24137.	1.3	24
35	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.	2.5	23
36	Hole Transport in Nonstoichiometric and Doped WÃ¼stite. Journal of Physical Chemistry C, 2012, 116, 17403-17413.	1.5	22

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37	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.	5.5	21
38	Breakdown of the Smallâ€Polaron Hopping Model in Higherâ€Order Spinels. Advanced Materials, 2020, 32, e2004490.	11.1	20
39	Site-directed electronic tunneling in a dissipative molecular environment. Journal of Chemical Physics, 2008, 129, 034501.	1.2	18
40	Electronic Properties of Pure and Fe-Doped Î²-Ni(OH)₂: New Insights Using Density Functional Theory with a Cluster Approach. Journal of Physical Chemistry C, 2016, 120, 12344-12350.	1.5	18
41	Dual Mechanisms: Hydrogen Transfer during Water Oxidation Catalysis of Pure and Fe-Doped Nickel Oxyhydroxide. Journal of Physical Chemistry C, 2017, 121, 16819-16824.	1.5	18
42	Communication: Nickel hydroxide as an exceptional deviation from the quantum size effect. Journal of Chemical Physics, 2018, 149, 141103.	1.2	17
43	Strong Band Gap Blueshift in Copper (I) Oxide Semiconductor via Bioinspired Route. Advanced Functional Materials, 2020, 30, 1910405.	7.8	17
44	Optimization of Niâ€'Coâ€'Feâ€Based Catalysts for Oxygen Evolution Reaction by Surface and Relaxation Phenomena Analysis. ChemSusChem, 2021, 14, 1737-1746.	3.6	17
45	Controlled electronic transport through branched molecular conductors. Molecular Physics, 2008, 106, 281-287.	0.8	15
46	Novel High-Throughput Screening Approach for Functional Metal/Oxide Interfaces. Journal of Chemical Theory and Computation, 2016, 12, 1572-1582.	2.3	15
47	Electronic Structure of Catalysis Intermediates by the G0W0 Approximation. Catalysis Letters, 2016, 146, 2009-2014.	1.4	15
48	Theoretical Investigation of Dielectric Materials for Twoâ€Dimensional Fieldâ€Effect Transistors. Advanced Functional Materials, 2020, 30, 1808544.	7.8	15
49	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.	5.2	15
50	Lateral Chemical Bonding in Two-Dimensional Transition-Metal Dichalcogenide Metal/Semiconductor Heterostructures. Journal of Physical Chemistry C, 2018, 122, 5401-5410.	1.5	14
51	Progress in understanding hematite electrochemistry through computational modeling. Computational Materials Science, 2019, 160, 411-419.	1.4	14
52	Manipulating electrochemical performance through doping beyond the solubility limit. Physical Chemistry Chemical Physics, 2016, 18, 16098-16105.	1.3	13
53	The Operando Optical Spectrum of Hematite during Water Splitting through a GWâ€"BSE Calculation. Journal of Chemical Theory and Computation, 2020, 16, 4857-4864.	2.3	13
54	On the nature of trapped states in an MoS₂ two-dimensional semiconductor with sulfur vacancies. Molecular Physics, 2019, 117, 2058-2068.	0.8	12

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55	Dipole-Induced Raman Enhancement Using Noncovalent Azobenzene-Functionalized Self-Assembled Monolayers on Graphene Terraces. ACS Applied Materials & Interfaces, 2021, 13, 10271-10278.	4.0	12
56	Water Oxidation Catalysis for NiOOH by a Metropolis Monte Carlo Algorithm. Journal of Chemical Theory and Computation, 2018, 14, 2380-2385.	2.3	11
57	Site-directed deep electronic tunneling through a molecular network. Journal of Chemical Physics, 2005, 123, 151101.	1.2	10
58	Efficient cationic agents for exfoliating two-dimensional nickel oxide sheets. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	10
59	Hydrogen transfer through different crystal phases of nickel oxy/hydroxide. Physical Chemistry Chemical Physics, 2018, 20, 25169-25178.	1.3	10
60	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.	1.2	10
61	Thermal rate constants for resonance-supporting reaction barriers by the flux averaging method. Chemical Physics Letters, 2003, 369, 232-239.	1.2	8
62	On the effect of nuclear bridge modes on donorâ€“acceptor electronic coupling in donorâ€“bridgeâ€“acceptor molecules. Chemical Physics, 2009, 358, 45-51.	0.9	8
63	Strategies to suppress cation vacancies in metal oxide alloys: consequences for solar energy conversion. Journal of Materials Science, 2015, 50, 5715-5722.	1.7	8
64	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.	1.5	8
65	The Effect of Fe and Co Additions on the Efficiency of NiOOH Catalyst Under Strain. ChemCatChem, 2020, 12, 2801-2806.	1.8	8
66	Bifunctional PGM-free metal organic framework-based electrocatalysts for alkaline electrolyzers: trends in the activity with different metal centers. Nanoscale, 2021, 13, 4576-4584.	2.8	8
67	The Effect of Covering Fe2O3 with a Ga2O3 Overlayer on Water Oxidation Catalysis. Catalysis Letters, 2017, 147, 2077-2082.	1.4	8
68	On the Interplay Between Oxygen Vacancies and Small Polarons in Manganese Iron Spinel Oxides. ACS Materials Au, 2022, 2, 269-277.	2.6	8
69	Metallic back-contact interface design in photoelectrochemical devices. Journal of Materials Chemistry C, 2016, 4, 8989-8996.	2.7	7
70	Practical Cluster Models for a Layered Î²-NiOOH Material. Materials, 2017, 10, 480.	1.3	7
71	The electronic structure of two-dimensional transition metal hydroxide monolayers and heterostructures. Solid State Ionics, 2018, 314, 149-155.	1.3	6
72	Materials with honeycomb structures for gate dielectrics in two-dimensional Field Effect Transistors â€“ An ab initio study. Ceramics International, 2019, 45, 9339-9347.	2.3	6

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73	Site-directed electronic tunneling through a vibrating molecular network. Journal of Chemical Physics, 2006, 125, 184703.	1.2	5
74	A quantum mechanical flux correlation approach to steady-state transport rates in molecular junctions. Chemical Physics, 2010, 370, 124-131.	0.9	5
75	Charge Transport Calculation along Twoâ€Dimensional Metal/Semiconductor/Metal Systems. Israel Journal of Chemistry, 2020, 60, 888-896.	1.0	5
76	Pathways for charge transport through material interfaces. Journal of Chemical Physics, 2020, 153, 024104.	1.2	5
77	Toward Ambitious Multiscale Modeling of Nanocrystal Catalysts for Water Splitting. ACS Energy Letters, 2020, 5, 2042-2044.	8.8	5
78	Transferable Classical Force Field for Pure and Mixed Metal Halide Perovskites Parameterized from First-Principles. Journal of Chemical Information and Modeling, 2022, 62, 6423-6435.	2.5	5
79	Electronic structure of Î²-NiOOH with hydrogen vacancies and implications for energy conversion applications. MRS Communications, 2017, 7, 206-213.	0.8	4
80	Revealing the Conducting Character of the Î²-NiOOH Catalyst through Defect Chemistry. Journal of Physical Chemistry C, 2019, 123, 18895-18904.	1.5	4
81	Enhanced Li-ion diffusion and electrochemical performance in strained-manganeseâ€“iron oxide coreâ€“shell nanoparticles. Journal of Chemical Physics, 2021, 155, 144702.	1.2	4
82	Simulations to Cover the Waterfront for Iron Oxide Catalysis. ChemPhysChem, 2022, 23, .	1.0	3
83	Electronic Structure Study of Various Transition Metal Oxide Spinels Reveals a Possible Design Strategy for Charge Transport Pathways. Journal of the Electrochemical Society, 2022, 169, 040542.	1.3	3
84	Thermal resonant tunneling rates by a generalized flux averaging method. Israel Journal of Chemistry, 2002, 42, 237-244.	1.0	2
85	Perovskite La_{0.3}Sr_{0.7}Fe_{0.7}Cr_{0.3}O_{3â”'}_{Î´} Catalysis Raises the Bar: Preventing Unwanted Nearâ€Surface Sr Segregation and SrCO₃ Precipitation. Advanced Theory and Simulations, 2022, 5, 2100173.	1.3	2
86	The effect of interlayer stacking arrangements in two dimensional NiOOH on water oxidation catalysis. Physical Chemistry Chemical Physics, 2022, 24, 854-860.	1.3	2
87	Changing your tune on catalytic efficiency: Tuning Cr concentration in La0.3Sr0.7Fe1-xCrxO3-Î´ perovskite as a cathode in solid oxide electrolysis cell. Computational Materials Science, 2022, 210, 111462.	1.4	2
88	Strain Controlling Catalytic Efficiency of Water Oxidation for Ni1â”'xFexOOH Alloy. Molecular Modeling and Simulation, 2021, , 1-23.	0.2	1
89	Method for assessing atomic sources of flicker noise in superconducting qubits. Npj Computational Materials, 2021, 7, .	3.5	1
90	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.	1.5	1

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91	Simultaneous propagation of different wavepackets driven by lasers. Chemical Physics Letters, 2006, 431, 169-173.	1.2	0
92	Electronic Charge Transport: Breakdown of the Smallâ€Polaron Hopping Model in Higherâ€Order Spinels (Adv. Mater. 49/2020). Advanced Materials, 2020, 32, 2070368.	11.1	0
93	Using Computers to Discover Materials That Generate Non-polluting Fuels. Frontiers for Young Minds, 0, 9, .	0.8	0
94	Advances in two dimensional NiOOH catalysis for the oxygen evolution reaction. , 0, , .		0
95	Optimization of Ni-Co-Fe-Based Catalysts for Oxygen Evolution Reaction by Theoretical Models. , 0, , .		0