

Benjamin Rudshhteyn

List of Publications by Year in descending order

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Version: 2024-02-01

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papers

1,329
citations

361413

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345221

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45
docs citations

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times ranked

2335
citing authors

#	ARTICLE	IF	CITATIONS
1	Facet-Dependent Photoelectrochemical Performance of TiO ₂ Nanostructures: An Experimental and Computational Study. <i>Journal of the American Chemical Society</i> , 2015, 137, 1520-1529.	13.7	242
2	CO ₂ Reduction Catalysts on Gold Electrode Surfaces Influenced by Large Electric Fields. <i>Journal of the American Chemical Society</i> , 2018, 140, 17643-17655.	13.7	103
3	Heterogenized Iridium Water-Oxidation Catalyst from a Silatrane Precursor. <i>ACS Catalysis</i> , 2016, 6, 5371-5377.	11.2	79
4	Interfacial Structure and Electric Field Probed by <i>in Situ</i> Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling. <i>Journal of Physical Chemistry C</i> , 2017, 121, 18674-18682.	3.1	77
5	On Achieving High Accuracy in Quantum Chemical Calculations of 3 <i>d</i> Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2346-2358.	5.3	62
6	Photoinduced electron transfer from rylene diimide radical anions and dianions to Re(bpy)(CO) ₃ using red and near-infrared light. <i>Chemical Science</i> , 2017, 8, 3821-3831.	7.4	57
7	Heterogenized Molecular Catalysts: Vibrational Sum-Frequency Spectroscopic, Electrochemical, and Theoretical Investigations. <i>Accounts of Chemical Research</i> , 2019, 52, 1289-1300.	15.6	53
8	Ultrafast Photoinduced Interfacial Proton Coupled Electron Transfer from CdSe Quantum Dots to 4,4'-Bipyridine. <i>Journal of the American Chemical Society</i> , 2016, 138, 884-892.	13.7	52
9	Stable Iridium(IV) Complexes of an Oxidation-Resistant Pyridine-Alkoxide Ligand: Highly Divergent Redox Properties Depending on the Isomeric Form Adopted. <i>Journal of the American Chemical Society</i> , 2015, 137, 7243-7250.	13.7	51
10	Orientation of Cyano-Substituted Bipyridine Re(I) <i>fac</i> -Tricarbonyl Electrocatalysts Bound to Conducting Au Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1657-1665.	3.1	46
11	Surface-Induced Anisotropic Binding of a Rhenium CO ₂ -Reduction Catalyst on Rutile TiO ₂ (110) Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 20970-20977.	3.1	44
12	Electrode-Ligand Interactions Dramatically Enhance CO ₂ Conversion to CO by the [Ni(cyclam)](PF ₆) ₂ Catalyst. <i>ACS Catalysis</i> , 2017, 7, 5282-5288.	11.2	43
13	Fundamental Role of Oxygen Stoichiometry in Controlling the Band Gap and Reactivity of Cupric Oxide Nanosheets. <i>Journal of the American Chemical Society</i> , 2016, 138, 10978-10985.	13.7	39
14	Synthesis and Characterization of Mono-, Di-, and Tri-Poly(ethylene glycol) Chlorine ₆ Conjugates for the Photokilling of Human Ovarian Cancer Cells. <i>Journal of Organic Chemistry</i> , 2012, 77, 10638-10647.	3.2	37
15	Water-Nucleophilic Attack Mechanism for the Cu ^{II} (pyalk) ₂ Water-Oxidation Catalyst. <i>ACS Catalysis</i> , 2018, 8, 7952-7960.	11.2	37
16	A full set of iridium(<i>iv</i>) pyridine-alkoxide stereoisomers: highly geometry-dependent redox properties. <i>Chemical Science</i> , 2017, 8, 1642-1652.	7.4	32
17	Molecular titanium-hydroxamate complexes as models for TiO ₂ surface binding. <i>Chemical Communications</i> , 2016, 52, 2972-2975.	4.1	30
18	Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal a Rotationally Fluid Adsorption State of \pm -Pinene on Silica. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12578-12589.	3.1	29

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19	Fabrication of Modularly Functionalizable Microcapsules Using Protein-Based Technologies. <i>ACS Biomaterials Science and Engineering</i> , 2016, 2, 1856-1861.	5.2	23
20	Electron-Induced Hole-Pair-Induced Vibrational Energy Relaxation of Rhenium Catalysts on Gold Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 406-412.	4.6	22
21	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3041-3054.	5.3	21
22	Thousandfold Enhancement of Photoreduction Lifetime in $\text{Re}(\text{bpy})(\text{CO})_3$ via Spin-Dependent Electron Transfer from a Perylene diimide Radical Anion Donor. <i>Journal of the American Chemical Society</i> , 2017, 139, 16466-16469.	13.7	20
23	Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Toward Benchmark Quantum Chemistry for Transition Metals. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2845-2862.	5.3	18
24	Assessment of DFT for Computing Sum Frequency Generation Spectra of an Epoxydiol and a Deuterated Isotopologue at Fused Silica/Vapor Interfaces. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1919-1927.	2.6	17
25	Collaboration between experiment and theory in solar fuels research. <i>Chemical Society Reviews</i> , 2019, 48, 1865-1873.	38.1	17
26	Inverse Design of a Catalyst for Aqueous CO/CO_2 Conversion Informed by the $\text{Ni}^{\text{II}}/\text{Ni}^{\text{I}}$ -Iminothiolate Complex. <i>Inorganic Chemistry</i> , 2018, 57, 15474-15480.	4.0	13
27	Dopant-Dependent SFG Response of Rhenium CO_2 Reduction Catalysts Chemisorbed on SrTiO_3 (100) Single Crystals. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13944-13952.	3.1	10
28	Multiple Stable Isoprene-Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. <i>Journal of the American Chemical Society</i> , 2020, 142, 10806-10813.	13.7	9
29	Orientations of nonlocal vibrational modes from combined experimental and theoretical sum frequency spectroscopy. <i>Chemical Physics Letters</i> , 2017, 683, 199-204.	2.6	8
30	Ultrafast photo-induced charge transfer of 1-naphthol and 2-naphthol to halocarbon solvents. <i>Chemical Physics Letters</i> , 2017, 683, 49-56.	2.6	8
31	Thermodynamic and Structural Factors That Influence the Redox Potentials of Tungsten-Alkylidyne Complexes. <i>ACS Catalysis</i> , 2017, 7, 6134-6143.	11.2	7
32	Inferring Protonation States of Hydroxamate Adsorbates on TiO_2 Surfaces. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11985-11990.	3.1	5
33	Theoretical Study of the Reaction Formaldehyde with Singlet Oxygen. Fragmentation of the C=N Bond, Ene Reaction and Other Processes. <i>Photochemistry and Photobiology</i> , 2014, 90, 431-438.	2.5	4
34	Computed Regioselectivity and Conjectured Biological Activity of Ene Reactions of Singlet Oxygen with the Natural Product Hyperforin. <i>Photochemistry and Photobiology</i> , 2017, 93, 626-631.	2.5	4
35	Is the Supporting Information the Venue for Reproducibility and Transparency?. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11425-11426.	2.6	2
36	Mechanistic study of CO/CO_2 conversion catalyzed by a biomimetic $\text{Ni}(\text{II})$ -Iminothiolate complex. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25555.	2.0	2

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37	Accurate Quantum Chemical Calculation of Ionization Potentials: Validation of the DFT-LOC Approach via a Large Data Set Obtained from Experiments and Benchmark Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2020, 16, 2109-2123.	5.3	2
38	Theoretical study of a nonpeptidic polydisulfide β -helix. Journal of Sulfur Chemistry, 2013, 34, 3-6.	2.0	1
39	Is the Supporting Information the Venue for Reproducibility and Transparency?. Journal of Physical Chemistry A, 2017, 121, 9680-9681.	2.5	1
40	Is the Supporting Information the Venue for Reproducibility and Transparency?. Journal of Physical Chemistry C, 2017, 121, 28212-28213.	3.1	1