# Benjamin Rudshteyn

List of Publications by Year
in descending order

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|---|---|---|---|
| 40<br>papers | 1,329<br>citations | 361413<br>20<br>h-index | 345221<br>36<br>g-index |
| 45<br>all docs | 45<br>docs citations | 45<br>times ranked | 2335<br>citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Toward Benchmark Quantum Chemistry for Transition Metals. Journal of Chemical Theory and Computation, 2022, 18, 2845-2862. | 5.3 | 18 |
| 2 | Multiple Stable Isopreneâ€“Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. Journal of the American Chemical Society, 2020, 142, 10806-10813. | 13.7 | 9 |
| 3 | 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 |
| 4 | Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2020, 16, 3041-3054. | 5.3 | 21 |
| 5 | Heterogenized Molecular Catalysts: Vibrational Sum-Frequency Spectroscopic, Electrochemical, and Theoretical Investigations. Accounts of Chemical Research, 2019, 52, 1289-1300. | 15.6 | 53 |
| 6 | On Achieving High Accuracy in Quantum Chemical Calculations of 3d Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. Journal of Chemical Theory and Computation, 2019, 15, 2346-2358. | 5.3 | 62 |
| 7 | Collaboration between experiment and theory in solar fuels research. Chemical Society Reviews, 2019, 48, 1865-1873. | 38.1 | 17 |
| 8 | Dopant-Dependent SFG Response of Rhenium CO<sub>2</sub> Reduction Catalysts Chemisorbed on SrTiO<sub>3</sub> (100) Single Crystals. Journal of Physical Chemistry C, 2018, 122, 13944-13952. | 3.1 | 10 |
| 9 | Mechanistic study of CO/CO 2 conversion catalyzed by a biomimetic Ni(II)â€iminothiolate complex. International Journal of Quantum Chemistry, 2018, 118, e25555. | 2.0 | 2 |
| 10 | Electronâ€“Hole-Pair-Induced Vibrational Energy Relaxation of Rhenium Catalysts on Gold Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 406-412. | 4.6 | 22 |
| 11 | Inverse Design of a Catalyst for Aqueous CO/CO<sub>2</sub> Conversion Informed by the Ni<sup>II</sup>â€“Iminothiolate Complex. Inorganic Chemistry, 2018, 57, 15474-15480. | 4.0 | 13 |
| 12 | CO<sub>2</sub> Reduction Catalysts on Gold Electrode Surfaces Influenced by Large Electric Fields. Journal of the American Chemical Society, 2018, 140, 17643-17655. | 13.7 | 103 |
| 13 | Water-Nucleophilic Attack Mechanism for the Cu<sup>II</sup>(pyalk)<sub>2</sub> Water-Oxidation Catalyst. ACS Catalysis, 2018, 8, 7952-7960. | 11.2 | 37 |
| 14 | Computed Regioselectivity and Conjectured Biological Activity of Ene Reactions of Singlet Oxygen with the Natural Product Hyperforin. Photochemistry and Photobiology, 2017, 93, 626-631. | 2.5 | 4 |
| 15 | Orientations of nonlocal vibrational modes from combined experimental and theoretical sum frequency spectroscopy. Chemical Physics Letters, 2017, 683, 199-204. | 2.6 | 8 |
| 16 | Photoinduced electron transfer from rylenediimide radical anions and dianions to Re(bpy)(CO)<sub>3</sub> using red and near-infrared light. Chemical Science, 2017, 8, 3821-3831. | 7.4 | 57 |
| 17 | Inferring Protonation States of Hydroxamate Adsorbates on TiO<sub>2</sub> Surfaces. Journal of Physical Chemistry C, 2017, 121, 11985-11990. | 3.1 | 5 |
| 18 | Ultrafast photo-induced charge transfer of 1-naphthol and 2-naphthol to halocarbon solvents. Chemical Physics Letters, 2017, 683, 49-56. | 2.6 | 8 |

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|---|---|---|---|
| 19 | Thousandfold Enhancement of Photoreduction Lifetime in Re(bpy)(CO)<sub>3</sub> via Spin-Dependent Electron Transfer from a Perylenediimide Radical Anion Donor. Journal of the American Chemical Society, 2017, 139, 16466-16469. | 13.7 | 20 |
| 20 | Interfacial Structure and Electric Field Probed by in Situ Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling. Journal of Physical Chemistry C, 2017, 121, 18674-18682. | 3.1 | 77 |
| 21 | Thermodynamic and Structural Factors That Influence the Redox Potentials of Tungstenâ€“Alkylidyne Complexes. ACS Catalysis, 2017, 7, 6134-6143. | 11.2 | 7 |
| 22 | Electrode-Ligand Interactions Dramatically Enhance CO<sub>2</sub> Conversion to CO by the [Ni(cyclam)](PF<sub>6</sub>)<sub>2</sub> Catalyst. ACS Catalysis, 2017, 7, 5282-5288. | 11.2 | 43 |
| 23 | A full set of iridium(<scp>iv</scp>) pyridine-alkoxide stereoisomers: highly geometry-dependent redox properties. Chemical Science, 2017, 8, 1642-1652. | 7.4 | 32 |
| 24 | Is the Supporting Information the Venue for Reproducibility and Transparency?. Journal of Physical Chemistry A, 2017, 121, 9680-9681. | 2.5 | 1 |
| 25 | Is the Supporting Information the Venue for Reproducibility and Transparency?. Journal of Physical Chemistry C, 2017, 121, 28212-28213. | 3.1 | 1 |
| 26 | Is the Supporting Information the Venue for Reproducibility and Transparency?. Journal of Physical Chemistry B, 2017, 121, 11425-11426. | 2.6 | 2 |
| 27 | Heterogenized Iridium Water-Oxidation Catalyst from a Silatrane Precursor. ACS Catalysis, 2016, 6, 5371-5377. | 11.2 | 79 |
| 28 | Fabrication of Modularly Functionalizable Microcapsules Using Protein-Based Technologies. ACS Biomaterials Science and Engineering, 2016, 2, 1856-1861. | 5.2 | 23 |
| 29 | Fundamental Role of Oxygen Stoichiometry in Controlling the Band Gap and Reactivity of Cupric Oxide Nanosheets. Journal of the American Chemical Society, 2016, 138, 10978-10985. | 13.7 | 39 |
| 30 | Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal a Rotationally Fluid Adsorption State of Î±-Pinene on Silica. Journal of Physical Chemistry C, 2016, 120, 12578-12589. | 3.1 | 29 |
| 31 | Surface-Induced Anisotropic Binding of a Rhenium CO<sub>2</sub>-Reduction Catalyst on Rutile TiO<sub>2</sub>(110) Surfaces. Journal of Physical Chemistry C, 2016, 120, 20970-20977. | 3.1 | 44 |
| 32 | Assessment of DFT for Computing Sum Frequency Generation Spectra of an Epoxydiol and a Deuterated Isotopologue at Fused Silica/Vapor Interfaces. Journal of Physical Chemistry B, 2016, 120, 1919-1927. | 2.6 | 17 |
| 33 | Ultrafast Photoinduced Interfacial Proton Coupled Electron Transfer from CdSe Quantum Dots to 4,4â€²-Bipyridine. Journal of the American Chemical Society, 2016, 138, 884-892. | 13.7 | 52 |
| 34 | Molecular titaniumâ€“hydroxamate complexes as models for TiO<sub>2</sub> surface binding. Chemical Communications, 2016, 52, 2972-2975. | 4.1 | 30 |
| 35 | Orientation of Cyano-Substituted Bipyridine Re(I) fac-Tricarbonyl Electrocatalysts Bound to Conducting Au Surfaces. Journal of Physical Chemistry C, 2016, 120, 1657-1665. | 3.1 | 46 |
| 36 | Facet-Dependent Photoelectrochemical Performance of TiO<sub>2</sub> Nanostructures: An Experimental and Computational Study. Journal of the American Chemical Society, 2015, 137, 1520-1529. | 13.7 | 242 |

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|---|---|---|---|
| 37 | Stable Iridium(IV) Complexes of an Oxidation-Resistant Pyridine-Alkoxide Ligand: Highly Divergent Redox Properties Depending on the Isomeric Form Adopted. Journal of the American Chemical Society, 2015, 137, 7243-7250. | 13.7 | 51 |
| 38 | Theoretical Study of the Reaction Formalhydrazone with Singlet Oxygen. Fragmentation of the C=N Bond, Ene Reaction and Other Processes. Photochemistry and Photobiology, 2014, 90, 431-438. | 2.5 | 4 |
| 39 | Theoretical study of a nonpeptidic polydisulfide Î±-helix<sup›â€</sup›. Journal of Sulfur Chemistry, 2013, 34, 3-6. | 2.0 | 1 |
| 40 | Synthesis and Characterization of Mono-, Di-, and Tri-Poly(ethylene glycol) Chlorin e<sub›6</sub› Conjugates for the Photokilling of Human Ovarian Cancer Cells. Journal of Organic Chemistry, 2012, 77, 10638-10647. | 3.2 | 37 |