

Bojana Ginovska

List of Publications by Year in descending order

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times ranked

1493
citing authors

#	ARTICLE	IF	CITATIONS
1	Analysis of Intermediates and Products from the Dehydrogenation of Mg(BH ₄) ₂ . Journal of Physical Chemistry A, 2022, 126, 444-452.	2.5	6
2	Exploring Detailed Reaction Pathways for Hydrogen Storage with Borohydrides Using DFT Calculations. Energy & Fuels, 2022, 36, 5513-5527.	5.1	2
3	Determinants of Selectivity for the Formation of Monocyclic and Bicyclic Products in Monoterpene Synthases. ACS Catalysis, 2022, 12, 7453-7469.	11.2	6
4	Splitting of multiple hydrogen molecules by bioinspired diniobium metal complexes: a DFT study. Dalton Transactions, 2021, 50, 840-849.	3.3	5
5	Mechanical coupling in the nitrogenase complex. PLoS Computational Biology, 2021, 17, e1008719.	3.2	8
6	Nickel-Sulfonate Mode of Substrate Binding for Forward and Reverse Reactions of Methyl-SCoM Reductase Suggest a Radical Mechanism Involving Long-Range Electron Transfer. Journal of the American Chemical Society, 2021, 143, 5481-5496.	13.7	12
7	De novo sequencing and native mass spectrometry revealed hetero-association of dirigent protein homologs and potential interacting proteins in Forsythia intermedia. Analyst, The, 2021, 146, 7670-7681.	3.5	0
8	Visualizing biomolecular electrostatics in virtual reality with UnityMol-APBS. Protein Science, 2020, 29, 237-246.	7.6	31
9	Tuning Catalytic Bias of Hydrogen Gas Producing Hydrogenases. Journal of the American Chemical Society, 2020, 142, 1227-1235.	13.7	55
10	Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair. Inorganic Chemistry, 2020, 59, 15295-15301.	4.0	8
11	A Positive Charge in the Outer Coordination Sphere of an Artificial Enzyme Increases CO ₂ Hydrogenation. Organometallics, 2020, 39, 1532-1544.	2.3	19
12	Chokepoints in Mechanical Coupling Associated with Allosteric Proteins: The Pyruvate Kinase Example. Biophysical Journal, 2019, 116, 1598-1608.	0.5	10
13	Structural characterization of the P1+ intermediate state of the P-cluster of nitrogenase. Journal of Biological Chemistry, 2018, 293, 9629-9635.	3.4	44
14	Solid-State NMR Identification of Intermolecular Interactions in Amelogenin Bound to Hydroxyapatite. Biophysical Journal, 2018, 115, 1666-1672.	0.5	12
15	Single-Amino Acid Modifications Reveal Additional Controls on the Proton Pathway of [FeFe]-Hydrogenase. Biochemistry, 2016, 55, 3165-3173.	2.5	29
16	The radical mechanism of biological methane synthesis by methyl-coenzyme M reductase. Science, 2016, 352, 953-958.	12.6	129
17	Graphene oxide membranes with high permeability and selectivity for dehumidification of air. Carbon, 2016, 106, 164-170.	10.3	54
18	Controlling Proton Delivery through Catalyst Structural Dynamics. Angewandte Chemie - International Edition, 2016, 55, 13509-13513.	13.8	48

#	ARTICLE	IF	CITATIONS
19	Achieving Reversible H ₂ /H ⁺ Interconversion at Room Temperature with Enzyme-Inspired Molecular Complexes: A Mechanistic Study. ACS Catalysis, 2016, 6, 6037-6049.	11.2	49
20	Investigating the role of chain and linker length on the catalytic activity of an H ₂ production catalyst containing a β -hairpin peptide. Journal of Coordination Chemistry, 2016, 69, 1730-1747.	2.2	15
21	Optimizing conditions for utilization of an H ₂ oxidation catalyst with outer coordination sphere functionalities. Dalton Transactions, 2016, 45, 9786-9793.	3.3	26
22	Heterolysis of H ₂ Across a Classical Lewis Pair, 2,6-Lutidine...BCl ₃ : Synthesis, Characterization, and Mechanism. Chemistry - A European Journal, 2015, 21, 15713-15719.	3.3	6
23	Photoswitching a molecular catalyst to regulate CO ₂ hydrogenation. Dalton Transactions, 2015, 44, 14854-14864.	3.3	17
24	Enzyme Design from the Bottom Up: An Active Nickel Electrocatalyst with a Structured Peptide Outer Coordination Sphere. Chemistry - A European Journal, 2014, 20, 1510-1514.	3.3	34
25	Beyond the Active Site: The Impact of the Outer Coordination Sphere on Electrocatalysts for Hydrogen Production and Oxidation. Accounts of Chemical Research, 2014, 47, 2621-2630.	15.6	152
26	Understanding ion-ion interactions in bulk and aqueous interfaces using molecular simulations. Faraday Discussions, 2013, 160, 151-160.	3.2	7
27	The Role of a Dipeptide Outer Coordination Sphere on H ₂ Production Catalysts: Influence on Catalytic Rates and Electron Transfer. Chemistry - A European Journal, 2013, 19, 1928-1941.	3.3	38
28	Note: Interionic potentials of mean force for Ca ²⁺ -Cl ⁻ in polarizable water. Journal of Chemical Physics, 2012, 136, .	3.0	12
29	Active Hydrogenation Catalyst with a Structured, Peptide-Based Outer-Coordination Sphere. ACS Catalysis, 2012, 2, 2114-2118.	11.2	14
30	The Role of Pendant Amines in the Breaking and Forming of Molecular Hydrogen Catalyzed by Nickel Complexes. Chemistry - A European Journal, 2012, 18, 6493-6506.	3.3	102
31	Analysis of the Activation and Heterolytic Dissociation of H ₂ by Frustrated Lewis Pairs: NH ₃ /BX ₃ (X = H, F, and Cl). Journal of Physical Chemistry A, 2012, 116, 7228-7237.	2.5	51
32	About the Barriers to Reaction of CCl ₄ with HFeOH and FeCl ₂ . Journal of Physical Chemistry A, 2011, 115, 8713-8720.	2.5	4
33	Modeling the Reaction of Fe Atoms with CCl ₄ . Journal of Physical Chemistry C, 2009, 113, 1830-1836.	3.1	11
34	The H ₂ O ₂ +OH ⁺ HO ₂ +H ₂ O reaction in aqueous solution from a charge-dependent continuum model of solvation. Journal of Chemical Physics, 2008, 129, 014506.	3.0	13
35	Charge-Dependent Cavity Radii for an Accurate Dielectric Continuum Model of Solvation with Emphasis on Ions: Aqueous Solutes with Oxo, Hydroxo, Amino, Methyl, Chloro, Bromo, and Fluoro Functionalities. Journal of Physical Chemistry A, 2008, 112, 10604-10613.	2.5	30
36	Reaction pathways and excited states in H ₂ O ₂ +OH ⁺ HO ₂ +H ₂ O: A new <i>ab initio</i> investigation. Journal of Chemical Physics, 2007, 127, 084309.	3.0	16

#	ARTICLE	IF	CITATIONS
37	CHAPTER 8. Biochemistry of Methyl-Coenzyme M Reductase. 2-Oxoglutarate-Dependent Oxygenases, 0, , 149-169.	0.8	6