

# Bojana Ginovska

## List of Publications by Year in descending order

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37  
papers

1,081  
citations

516710

16  
h-index

414414

32  
g-index

38  
all docs

38  
docs citations

38  
times ranked

1493  
citing authors

#	ARTICLE	IF	CITATIONS
1	Beyond the Active Site: The Impact of the Outer Coordination Sphere on Electrocatalysts for Hydrogen Production and Oxidation. <i>Accounts of Chemical Research</i> , 2014, 47, 2621-2630.	15.6	152
2	The radical mechanism of biological methane synthesis by methyl-coenzyme M reductase. <i>Science</i> , 2016, 352, 953-958.	12.6	129
3	The Role of Pendant Amines in the Breaking and Forming of Molecular Hydrogen Catalyzed by Nickel Complexes. <i>Chemistry - A European Journal</i> , 2012, 18, 6493-6506.	3.3	102
4	Tuning Catalytic Bias of Hydrogen Gas Producing Hydrogenases. <i>Journal of the American Chemical Society</i> , 2020, 142, 1227-1235.	13.7	55
5	Graphene oxide membranes with high permeability and selectivity for dehumidification of air. <i>Carbon</i> , 2016, 106, 164-170.	10.3	54
6	Analysis of the Activation and Heterolytic Dissociation of H <sub>2</sub> by Frustrated Lewis Pairs: NH <sub>3</sub> /BX <sub>3</sub> (X = H, F, and Cl). <i>Journal of Physical Chemistry A</i> , 2012, 116, 7228-7237.	2.5	51
7	Achieving Reversible H <sub>2</sub> /H <sup>+</sup> Interconversion at Room Temperature with Enzyme-Inspired Molecular Complexes: A Mechanistic Study. <i>ACS Catalysis</i> , 2016, 6, 6037-6049.	11.2	49
8	Controlling Proton Delivery through Catalyst Structural Dynamics. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 13509-13513.	13.8	48
9	Structural characterization of the P1+ intermediate state of the P-cluster of nitrogenase. <i>Journal of Biological Chemistry</i> , 2018, 293, 9629-9635.	3.4	44
10	The Role of a Dipeptide Outer Coordination Sphere on H <sub>2</sub> Production Catalysts: Influence on Catalytic Rates and Electron Transfer. <i>Chemistry - A European Journal</i> , 2013, 19, 1928-1941.	3.3	38
11	Enzyme Design from the Bottom Up: An Active Nickel Electrocatalyst with a Structured Peptide Outer Coordination Sphere. <i>Chemistry - A European Journal</i> , 2014, 20, 1510-1514.	3.3	34
12	Visualizing biomolecular electrostatics in virtual reality with UnityMolAPBS. <i>Protein Science</i> , 2020, 29, 237-246.	7.6	31
13	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. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10604-10613.	2.5	30
14	Single-Amino Acid Modifications Reveal Additional Controls on the Proton Pathway of [FeFe]-Hydrogenase. <i>Biochemistry</i> , 2016, 55, 3165-3173.	2.5	29
15	Optimizing conditions for utilization of an H <sub>2</sub> oxidation catalyst with outer coordination sphere functionalities. <i>Dalton Transactions</i> , 2016, 45, 9786-9793.	3.3	26
16	A Positive Charge in the Outer Coordination Sphere of an Artificial Enzyme Increases CO <sub>2</sub> Hydrogenation. <i>Organometallics</i> , 2020, 39, 1532-1544.	2.3	19
17	Photoswitching a molecular catalyst to regulate CO <sub>2</sub> hydrogenation. <i>Dalton Transactions</i> , 2015, 44, 14854-14864.	3.3	17
18	Reaction pathways and excited states in H <sub>2</sub> O <sub>2</sub> +OH <sup>+</sup> HO <sub>2</sub> +H <sub>2</sub> O: A new <i>ab initio</i> investigation. <i>Journal of Chemical Physics</i> , 2007, 127, 084309.	3.0	16

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19	Investigating the role of chain and linker length on the catalytic activity of an H <sub>2</sub> production catalyst containing a $\beta$ -hairpin peptide. <i>Journal of Coordination Chemistry</i> , 2016, 69, 1730-1747.	2.2	15
20	Active Hydrogenation Catalyst with a Structured, Peptide-Based Outer-Coordination Sphere. <i>ACS Catalysis</i> , 2012, 2, 2114-2118.	11.2	14
21	The H <sub>2</sub> O <sub>2</sub> +OH <sup>-</sup> →HO <sub>2</sub> +H <sub>2</sub> O reaction in aqueous solution from a charge-dependent continuum model of solvation. <i>Journal of Chemical Physics</i> , 2008, 129, 014506.	3.0	13
22	Note: Interionic potentials of mean force for Ca <sup>2+</sup> -Cl <sup>-</sup> in polarizable water. <i>Journal of Chemical Physics</i> , 2012, 136, .	3.0	12
23	Solid-State NMR Identification of Intermolecular Interactions in Amelogenin Bound to Hydroxyapatite. <i>Biophysical Journal</i> , 2018, 115, 1666-1672.	0.5	12
24	Nickel <sup>II</sup> -Sulfonate Mode of Substrate Binding for Forward and Reverse Reactions of Methyl-SCoM Reductase Suggest a Radical Mechanism Involving Long-Range Electron Transfer. <i>Journal of the American Chemical Society</i> , 2021, 143, 5481-5496.	13.7	12
25	Modeling the Reaction of Fe Atoms with CCl <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , 2009, 113, 1830-1836.	3.1	11
26	Chokepoints in Mechanical Coupling Associated with Allosteric Proteins: The Pyruvate Kinase Example. <i>Biophysical Journal</i> , 2019, 116, 1598-1608.	0.5	10
27	Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair. <i>Inorganic Chemistry</i> , 2020, 59, 15295-15301.	4.0	8
28	Mechanical coupling in the nitrogenase complex. <i>PLoS Computational Biology</i> , 2021, 17, e1008719.	3.2	8
29	Understanding ion-ion interactions in bulk and aqueous interfaces using molecular simulations. <i>Faraday Discussions</i> , 2013, 160, 151-160.	3.2	7
30	Heterolysis of H <sub>2</sub> Across a Classical Lewis Pair, 2,6-Lutidine...BCl <sub>3</sub> : Synthesis, Characterization, and Mechanism. <i>Chemistry - A European Journal</i> , 2015, 21, 15713-15719.	3.3	6
31	CHAPTER 8. Biochemistry of Methyl-Coenzyme M Reductase. 2-Oxoglutarate-Dependent Oxygenases, 0, , 149-169.	0.8	6
32	Analysis of Intermediates and Products from the Dehydrogenation of Mg(BH <sub>4</sub> ) <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2022, 126, 444-452.	2.5	6
33	Determinants of Selectivity for the Formation of Monocyclic and Bicyclic Products in Monoterpene Synthases. <i>ACS Catalysis</i> , 2022, 12, 7453-7469.	11.2	6
34	Splitting of multiple hydrogen molecules by bioinspired diniobium metal complexes: a DFT study. <i>Dalton Transactions</i> , 2021, 50, 840-849.	3.3	5
35	About the Barriers to Reaction of CCl <sub>4</sub> with HFeOH and FeCl <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2011, 115, 8713-8720.	2.5	4
36	Exploring Detailed Reaction Pathways for Hydrogen Storage with Borohydrides Using DFT Calculations. <i>Energy &amp; Fuels</i> , 2022, 36, 5513-5527.	5.1	2

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37	<i>De novo</i> sequencing and native mass spectrometry revealed hetero-association of dirigent protein homologs and potential interacting proteins in <i>Forsythia</i> — <i>intermedia</i> . <i>Analyst</i> , The, 2021, 146, 7670-7681.	3.5	0