

# Bess Vlasisavljevich

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/509570/publications.pdf>

Version: 2024-02-01

48  
papers

2,686  
citations

236612

25  
h-index

205818

48  
g-index

51  
all docs

51  
docs citations

51  
times ranked

3956  
citing authors

#	ARTICLE	IF	CITATIONS
1	Cooperative insertion of CO <sub>2</sub> in diamine-appended metal-organic frameworks. <i>Nature</i> , 2015, 519, 303-308.	13.7	1,026
2	On the Nature of Actinide- and Lanthanide-Metal Bonds in Heterobimetallic Compounds. <i>Chemistry - A European Journal</i> , 2011, 17, 8424-8433.	1.7	112
3	Defining the Macromolecules of Tomorrow through Synergistic Sustainable Polymer Research. <i>Chemical Reviews</i> , 2022, 122, 6322-6373.	23.0	99
4	Understanding the Structure and Formation of Uranyl Peroxide Nanoclusters by Quantum Chemical Calculations. <i>Journal of the American Chemical Society</i> , 2010, 132, 14503-14508.	6.6	98
5	Nuclear Energy Gradients for Internally Contracted Complete Active Space Second-Order Perturbation Theory: Multistate Extensions. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3781-3787.	2.3	97
6	Investigations of the Electronic Structure of Arene-Bridged Diuranium Complexes. <i>Organometallics</i> , 2013, 32, 1341-1352.	1.1	87
7	Multireference Electron Correlation Methods: Journeys along Potential Energy Surfaces. <i>Chemical Reviews</i> , 2020, 120, 5878-5909.	23.0	86
8	Critical Factors Driving the High Volumetric Uptake of Methane in Cu <sub>3</sub> (btc) <sub>2</sub> . <i>Journal of the American Chemical Society</i> , 2015, 137, 10816-10825.	6.6	73
9	Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of <i>n</i> -Butane. <i>Journal of the American Chemical Society</i> , 2016, 138, 4739-4756.	6.6	72
10	Metal-ligand covalency enables room temperature molecular qubit candidates. <i>Chemical Science</i> , 2019, 10, 6707-6714.	3.7	50
11	Divergent Adsorption-Dependent Luminescence of Amino-Functionalized Lanthanide Metal-Organic Frameworks for Highly Sensitive NO <sub>2</sub> Sensors. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3362-3368.	2.1	50
12	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of <i>n</i> -Alkanes on Brønsted Acid Sites in Zeolites. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10427-10438.	1.5	48
13	CO <sub>2</sub> induced phase transitions in diamine-appended metal-organic frameworks. <i>Chemical Science</i> , 2015, 6, 5177-5185.	3.7	45
14	Cation Templating and Electronic Structure Effects in Uranyl Cage Clusters Probed by the Isolation of Peroxide-Bridged Uranyl Dimers. <i>Inorganic Chemistry</i> , 2015, 54, 4445-4455.	1.9	44
15	Combined Triple and Double Bonds to Uranium: The N <sub>2</sub> U <sub>2</sub> H Uranimine Nitride Molecule Prepared in Solid Argon. <i>Inorganic Chemistry</i> , 2011, 50, 3826-3831.	1.9	43
16	Probing the mechanism of CO <sub>2</sub> capture in diamine-appended metal-organic frameworks using measured and simulated X-ray spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21448-21457.	1.3	43
17	Uranium(III)-carbon multiple bonding supported by arene $\pi$ -bonding in mixed-valence hexauranium nanometre-scale rings. <i>Nature Communications</i> , 2018, 9, 2097.	5.8	43
18	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M <sub>2</sub> (dobdc) Metal-Organic Frameworks. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4139-4151.	1.1	41

#	ARTICLE	IF	CITATIONS
19	Transformation of the coordination complex [Co(C <sub>3</sub> S <sub>5</sub> ) <sub>2</sub> ] <sup>2+</sup> from a molecular magnet to a potential qubit. <i>Chemical Science</i> , 2016, 7, 6160-6166.	3.7	40
20	Buffered Coordination Modulation as a Means of Controlling Crystal Morphology and Molecular Diffusion in an Anisotropic Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2021, 143, 5044-5052.	6.6	35
21	Understanding Small-Molecule Interactions in Metal-Organic Frameworks: Coupling Experiment with Theory. <i>Advanced Materials</i> , 2015, 27, 5785-5796.	11.1	33
22	Hopping Transport and Rectifying Behavior in Long Donor-Acceptor Molecular Wires. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26485-26497.	1.5	32
23	Self-Assembly of Uranyl-Peroxide Nanocapsules in Basic Peroxidic Environments. <i>Chemistry - A European Journal</i> , 2016, 22, 8571-8578.	1.7	32
24	Infrared Spectra of Small Insertion and Methylidene Complexes in Reactions of Laser-Ablated Nickel Atoms with Halomethanes. <i>Organometallics</i> , 2009, 28, 5623-5632.	1.1	31
25	Infrared Spectra and Electronic Structure Calculations for NN Complexes with U, UN, and NUN in Solid Argon, Neon, and Nitrogen. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5289-5303.	1.1	25
26	Biased Spin-State Energetics of Fe(II) Molecular Complexes within Density-Functional Theory and the Linear-Response Hubbard <i>U</i> -Correction. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6755-6762.	2.3	23
27	Uranyl-Peroxide Nanocapsules in Aqueous Solution: Force Field Development and First Applications. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24730-24740.	1.5	22
28	Improved Spin-State Energy Differences of Fe(II) Molecular and Crystalline Complexes <i>via</i> the Hubbard <i>U</i> -Corrected Density. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2807-2816.	2.3	22
29	Synthesis and Characterization of the First <sup>2</sup> D Neptunyl Structure Stabilized by Side-on Cation-Cation Interactions. <i>Chemistry - A European Journal</i> , 2013, 19, 2937-2941.	1.7	21
30	Infrared Spectra and Electronic Structure Calculations for the NUN(NN) <sup>5+</sup> and NU(NN) <sup>6+</sup> Complexes in Solid Argon. <i>Inorganic Chemistry</i> , 2013, 52, 9989-9993.	1.9	21
31	Detection and Electronic Structure of Naked Actinide Complexes: Rhombic-Ring (AnN) <sub>2</sub> Molecules Stabilized by Delocalized $\pi$ -Bonding. <i>Journal of the American Chemical Society</i> , 2016, 138, 893-905.	6.6	20
32	Volatilities of Actinide and Lanthanide <i>N</i> , <i>N</i> -Dimethylaminodiboranate Chemical Vapor Deposition Precursors: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23194-23200.	1.5	19
33	Effects of Pore and Cage Topology on the Thermodynamics of <i>n</i> -Alkane Adsorption at Brønsted Protons in Zeolites at High Temperature. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1618-1638.	1.5	17
34	Modifying the luminescent properties of a Cu( <i>scpd</i> ) diphosphine complex using ligand-centered reactions in single crystals. <i>Chemical Communications</i> , 2020, 56, 9110-9113.	2.2	17
35	U and P <sub>4</sub> Reaction Products: A Quantum Chemical and Matrix Isolation Spectroscopic Investigation. <i>Inorganic Chemistry</i> , 2010, 49, 9230-9235.	1.9	16
36	Actinide arene-metalates: ion pairing effects on the electronic structure of unsupported uranium-arene sandwich complexes. <i>Chemical Science</i> , 2021, 12, 13360-13372.	3.7	13

#	ARTICLE	IF	CITATIONS
37	Electronic structure of SmO and SmOâ™ via slow photoelectron velocity-map imaging spectroscopy and spin-orbit CASPT2 calculations. <i>Journal of Chemical Physics</i> , 2017, 147, 234311.	1.2	12
38	Structural Characterization of the [CuOR] <sup>2+</sup> Core. <i>Journal of the American Chemical Society</i> , 2021, 143, 3295-3299.	6.6	12
39	CASPT2 molecular geometries of Fe( <sup>ii</sup> ) spin-crossover complexes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1390-1398.	1.3	12
40	Sulfur-Containing Analogues of the Reactive [CuOH] <sup>2+</sup> Core. <i>Inorganic Chemistry</i> , 2021, 60, 5217-5223.	1.9	11
41	Turning a New Leaf on Metal-TMC Chemistry: Ni <sup>II</sup> (TMC) Acetylides. <i>Inorganic Chemistry</i> , 2015, 54, 10058-10064.	1.9	10
42	Homoleptic uranium and lanthanide phosphinodiboranates. <i>Chemical Communications</i> , 2018, 54, 5602-5605.	2.2	8
43	Isolation of ligand-centered borocations in molybdenum complexes containing a triaminoborane-bridged diphosphorus ligand. <i>Dalton Transactions</i> , 2019, 48, 3777-3785.	1.6	7
44	On the Spatial Design of Co-Fed Amines for Selective Dehydration of Methyl Lactate to Acrylates. <i>ACS Catalysis</i> , 2021, 11, 5718-5735.	5.5	6
45	Computational Spectroscopy of the Crâ€“Cr Bond in Coordination Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 19219-19225.	1.9	5
46	Orbital energy mismatch engenders high-spin ground states in heterobimetallic complexes. <i>Chemical Science</i> , 2020, 11, 9971-9977.	3.7	4
47	Ligand Effects on Decarbonylation of Palladium-Acyl Complexes. <i>Organometallics</i> , 2020, 39, 3992-3998.	1.1	2
48	Prediction of Molecular Properties Including Symmetry from Quantum-Based Molecular Structural Formulas, VIF. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9784-9795.	1.1	1