Bess Vlaisavljevich

List of Publications by Year
in descending order

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48 papers	2,686 citations	236833 25 h-index	206029 48 g-index
51 all docs	51 docs citations	51 times ranked	3956 citing authors

#	Article	IF	Citations
1	CASPT2 molecular geometries of Fe(<scp>ii</scp>) spin-crossover complexes. Physical Chemistry Chemical Physics, 2022, 24, 1390-1398.	1.3	12
2	Defining the Macromolecules of Tomorrow through Synergistic Sustainable Polymer Research. Chemical Reviews, 2022, 122, 6322-6373.	23.0	99
3	Structural Characterization of the [CuOR]²⁺ Core. Journal of the American Chemical Society, 2021, 143, 3295-3299.	6.6	12
4	Sulfur-Containing Analogues of the Reactive [CuOH]²⁺ Core. Inorganic Chemistry, 2021, 60, 5217-5223.	1.9	11
5	Buffered Coordination Modulation as a Means of Controlling Crystal Morphology and Molecular Diffusion in an Anisotropic Metalâ€“Organic Framework. Journal of the American Chemical Society, 2021, 143, 5044-5052.	6.6	35
6	Improved Spin-State Energy Differences of Fe(II) Molecular and Crystalline Complexes via the Hubbard U-Corrected Density. Journal of Chemical Theory and Computation, 2021, 17, 2807-2816.	2.3	22
7	On the Spatial Design of Co-Fed Amines for Selective Dehydration of Methyl Lactate to Acrylates. ACS Catalysis, 2021, 11, 5718-5735.	5.5	6
8	Actinide arene-metalates: ion pairing effects on the electronic structure of unsupported uraniumâ€“arenide sandwich complexes. Chemical Science, 2021, 12, 13360-13372.	3.7	13
9	Computational Spectroscopy of the Crâ€“Cr Bond in Coordination Complexes. Inorganic Chemistry, 2021, 60, 19219-19225.	1.9	5
10	Biased Spin-State Energetics of Fe(II) Molecular Complexes within Density-Functional Theory and the Linear-Response Hubbard U Correction. Journal of Chemical Theory and Computation, 2020, 16, 6755-6762.	2.3	23
11	Orbital energy mismatch engenders high-spin ground states in heterobimetallic complexes. Chemical Science, 2020, 11, 9971-9977.	3.7	4
12	Ligand Effects on Decarbonylation of Palladium-Acyl Complexes. Organometallics, 2020, 39, 3992-3998.	1.1	2
13	Divergent Adsorption-Dependent Luminescence of Amino-Functionalized Lanthanide Metalâ€“Organic Frameworks for Highly Sensitive NO₂ Sensors. Journal of Physical Chemistry Letters, 2020, 11, 3362-3368.	2.1	50
14	Multireference Electron Correlation Methods: Journeys along Potential Energy Surfaces. Chemical Reviews, 2020, 120, 5878-5909.	23.0	86
15	Modifying the luminescent properties of a Cu(<scp>i</scp>) diphosphine complex using ligand-centered reactions in single crystals. Chemical Communications, 2020, 56, 9110-9113.	2.2	17
16	Metalâ€“ligand covalency enables room temperature molecular qubit candidates. Chemical Science, 2019, 10, 6707-6714.	3.7	50
17	Isolation of ligand-centered borocations in molybdenum complexes containing a triaminoborane-bridged diphosphorus ligand. Dalton Transactions, 2019, 48, 3777-3785.	1.6	7
18	Uranium(III)-carbon multiple bonding supported by arene Î´-bonding in mixed-valence hexauranium nanometre-scale rings. Nature Communications, 2018, 9, 2097.	5.8	43

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19	Homoleptic uranium and lanthanide phosphinodiboranates. Chemical Communications, 2018, 54, 5602-5605.	2.2	8
20	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M₂(dobdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry A, 2017, 121, 4139-4151.	1.1	41
21	Effects of Pore and Cage Topology on the Thermodynamics of n-Alkane Adsorption at BrÃ¸nsted Protons in Zeolites at High Temperature. Journal of Physical Chemistry C, 2017, 121, 1618-1638.	1.5	17
22	Electronic structure of SmO and SmOâ^' via slow photoelectron velocity-map imaging spectroscopy and spin-orbit CASPT2 calculations. Journal of Chemical Physics, 2017, 147, 234311.	1.2	12
23	Selfâ€Assembly of Uranylâ€“Peroxide Nanocapsules in Basic Peroxidic Environments. Chemistry - A European Journal, 2016, 22, 8571-8578.	1.7	32
24	Transformation of the coordination complex [Co(C₃S₅)₂]^{2â^'} from a molecular magnet to a potential qubit. Chemical Science, 2016, 7, 6160-6166.	3.7	40
25	Nuclear Energy Gradients for Internally Contracted Complete Active Space Second-Order Perturbation Theory: Multistate Extensions. Journal of Chemical Theory and Computation, 2016, 12, 3781-3787.	2.3	97
26	Detection and Electronic Structure of Naked Actinide Complexes: Rhombic-Ring (AnN)2 Molecules Stabilized by Delocalized Ï€-Bonding. Journal of the American Chemical Society, 2016, 138, 893-905.	6.6	20
27	Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of n-Butane. Journal of the American Chemical Society, 2016, 138, 4739-4756.	6.6	72
28	Understanding Smallâ€Molecule Interactions in Metalâ€“Organic Frameworks: Coupling Experiment with Theory. Advanced Materials, 2015, 27, 5785-5796.	11.1	33
29	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of n-Alkanes on BrÃ¸nsted Acid Sites in Zeolites. Journal of Physical Chemistry C, 2015, 119, 10427-10438.	1.5	48
30	Turning a New Leaf on Metal-TMC Chemistry: Ni^{II}(TMC) Acetylides. Inorganic Chemistry, 2015, 54, 10058-10064.	1.9	10
31	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	13.7	1,026
32	CO₂ induced phase transitions in diamine-appended metalâ€“organic frameworks. Chemical Science, 2015, 6, 5177-5185.	3.7	45
33	Cation Templating and Electronic Structure Effects in Uranyl Cage Clusters Probed by the Isolation of Peroxide-Bridged Uranyl Dimers. Inorganic Chemistry, 2015, 54, 4445-4455.	1.9	44
34	Probing the mechanism of CO₂ capture in diamine-appended metalâ€“organic frameworks using measured and simulated X-ray spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 21448-21457.	1.3	43
35	Critical Factors Driving the High Volumetric Uptake of Methane in Cu₃(btc)₂. Journal of the American Chemical Society, 2015, 137, 10816-10825.	6.6	73
36	Hopping Transport and Rectifying Behavior in Long Donorâ€“Acceptor Molecular Wires. Journal of Physical Chemistry C, 2014, 118, 26485-26497.	1.5	32

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37	Uranylâ€“Peroxide Nanocapsules in Aqueous Solution: Force Field Development and First Applications. Journal of Physical Chemistry C, 2014, 118, 24730-24740.	1.5	22
38	Infrared Spectra and Electronic Structure Calculations for NN Complexes with U, UN, and NUN in Solid Argon, Neon, and Nitrogen. Journal of Physical Chemistry A, 2014, 118, 5289-5303.	1.1	25
39	Synthesis and Characterization of the First 2â€‰D Neptunyl Structure Stabilized by Sideâ€on Cationâ€“Cation Interactions. Chemistry - A European Journal, 2013, 19, 2937-2941.	1.7	21
40	Investigations of the Electronic Structure of Arene-Bridged Diuranium Complexes. Organometallics, 2013, 32, 1341-1352.	1.1	87
41	Infrared Spectra and Electronic Structure Calculations for the NUN(NN)_{1â€“5} and NU(NN)_{1â€“6} Complexes in Solid Argon. Inorganic Chemistry, 2013, 52, 9989-9993.	1.9	21
42	Volatilities of Actinide and Lanthanide N,N-Dimethylaminodiboranate Chemical Vapor Deposition Precursors: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 23194-23200.	1.5	19
43	Combined Triple and Double Bonds to Uranium: The Nâ‰¡Uâ•Nâˆ’H Uranimine Nitride Molecule Prepared in Solid Argon. Inorganic Chemistry, 2011, 50, 3826-3831.	1.9	43
44	On the Nature of Actinideâ€“ and Lanthanideâ€“Metal Bonds in Heterobimetallic Compounds. Chemistry - A European Journal, 2011, 17, 8424-8433.	1.7	112
45	U and P4Reaction Products: A Quantum Chemical and Matrix Isolation Spectroscopic Investigation. Inorganic Chemistry, 2010, 49, 9230-9235.	1.9	16
46	Understanding the Structure and Formation of Uranyl Peroxide Nanoclusters by Quantum Chemical Calculations. Journal of the American Chemical Society, 2010, 132, 14503-14508.	6.6	98
47	Infrared Spectra of Small Insertion and Methylidene Complexes in Reactions of Laser-Ablated Nickel Atoms with Halomethanes. Organometallics, 2009, 28, 5623-5632.	1.1	31
48	Prediction of Molecular Properties Including Symmetry from Quantum-Based Molecular Structural Formulas, VIF. Journal of Physical Chemistry A, 2008, 112, 9784-9795.	1.1	1