

Jun-Bo Lu

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Ultra-Efficient Americium/Lanthanide Separation through Oxidation State Control. <i>Journal of the American Chemical Society</i> , 2022, 144, 6383-6389.	13.7	33
2	On the highest oxidation states of the actinoids in AnO_4 molecules ($\text{An} = \text{Ac}$). <i>Overlock</i>	9.3	0
3	Coordination Sphere of Lanthanide Aqua Ions Resolved with Ab Initio Molecular Dynamics and X-ray Absorption Spectroscopy. <i>Inorganic Chemistry</i> , 2021, 60, 3117-3130.	4.0	33
4	Norm-Conserving Pseudopotentials and Basis Sets to Explore Actinide Chemistry in Complex Environments. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3360-3371.	5.3	19
5	Electronic Structure and Spectroscopic Properties of Group-7 Tri-Oxo-Halides MO_3X ($\text{M} = \text{Tj}$). <i>Overlock</i>	4.0	3
6	Norm-Conserving Pseudopotentials and Basis Sets To Explore Lanthanide Chemistry in Complex Environments. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5987-5997.	5.3	46
7	The σ -Dative Bonding in a Uranium-Cobalt Heterobimetallic Complex for Efficient Nitrogen Fixation. <i>Inorganic Chemistry</i> , 2019, 58, 7433-7439.	4.0	19
8	N_2 Reduction on Fe-Based Complexes with Different Supporting Main-Group Elements: Critical Roles of Anchor and Peripheral Ligands. <i>Small Methods</i> , 2019, 3, 1800340.	8.6	17
9	Lanthanides with Unusually Low Oxidation States in the PrB_3 and PrB_4 Boride Clusters. <i>Inorganic Chemistry</i> , 2019, 58, 411-418.	4.0	39
10	Electronic Structure and Bonding Situation in M_2O_2 ($\text{M} = \text{Be, Mg, Ca}$) Rhombic Clusters. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2816-2822.	2.5	34
11	Relativity-Induced Bonding Pattern Change in Coinage Metal Dimers M_2 ($\text{M} = \text{Cu, Ag, Au, Rg}$). <i>Inorganic Chemistry</i> , 2018, 57, 5499-5506.	4.0	12
12	Efficient Nitrogen Fixation via a Redox-Flexible Single-Iron Site with Reverse-Dative Iron-Boron Bonding. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4530-4537.	2.5	23
13	On the Upper Limits of Oxidation States in Chemistry. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3242-3245.	13.8	46
14	Polarizable force field parameterization and theoretical simulations of $\text{ThCl}_4 \cdot \text{LiCl}$ molten salts. <i>Journal of Computational Chemistry</i> , 2018, 39, 2432-2438.	3.3	11
15	A supramolecular radical cation: folding-enhanced electrostatic effect for promoting radical-mediated oxidation. <i>Chemical Science</i> , 2018, 9, 5015-5020.	7.4	21
16	Pentavalent Lanthanide Compounds: Formation and Characterization of Praseodymium(V) Oxides. <i>Angewandte Chemie</i> , 2016, 128, 7010-7014.	2.0	10
17	Pentavalent Lanthanide Compounds: Formation and Characterization of Praseodymium(V) Oxides. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 6896-6900.	13.8	66
18	How Much Can Density Functional Approximations (DFA) Fail? The Extreme Case of the FeO_4 Species. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1525-1533.	5.3	33

#	ARTICLE	IF	CITATIONS
19	Experimental and theoretical identification of the Fe(^{vii}) oxidation state in FeO ₄ ²⁻ . Physical Chemistry Chemical Physics, 2016, 18, 31125-31131.	2.8	18