Rebecca K Carlson

List of Publications by Year
in descending order

24 papers	3,229 citations	567281 15 h-index	526287 27 g-index
30 all docs	30 docs citations	30 times ranked	3777 citing authors

#	Article	IF	Citations
1	Spectroscopic and electrochemical characterization of a Pr⁴⁺ imidophosphorane complex and the redox chemistry of Nd³⁺ and Dy³⁺ complexes. Dalton Transactions, 2022, 51, 6696-6706.	3.3	11
2	Mechanistic Study of the Production of NO_x Gases from the Reaction of Copper with Nitric Acid. Inorganic Chemistry, 2020, 59, 16833-16842.	4.0	1
3	Tight-Binding Modeling of Uranium in an Aqueous Environment. Journal of Chemical Theory and Computation, 2020, 16, 3073-3083.	5.3	6
4	On-Top Ratio for Atoms and Molecules. Journal of Physical Chemistry A, 2019, 123, 8294-8304.	2.5	2
5	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
6	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. Accounts of Chemical Research, 2017, 50, 66-73.	15.6	232
7	On-Top Pair Density as a Measure of Leftâ€“Right Correlation in Bond Breaking. Journal of Physical Chemistry A, 2017, 121, 5540-5547.	2.5	13
8	Synthesis and characterization of triply-bonded titanium-iron complexes supported by 2-(diphenylphosphino)pyrrolide ligands. Inorganica Chimica Acta, 2017, 460, 43-48.	2.4	10
9	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
10	Computationally Guided Discovery of a Catalytic Cobalt-Decorated Metalâ€“Organic Framework for Ethylene Dimerization. Journal of Physical Chemistry C, 2016, 120, 23576-23583.	3.1	78
11	Separated-pair approximation and separated-pair pair-density functional theory. Chemical Science, 2016, 7, 2399-2413.	7.4	47
12	Structure and bonding of group 4-nickel heterobimetallics supported by 2-(diphenylphosphino)pyrrolide ligands. Dalton Transactions, 2016, 45, 9892-9901.	3.3	24
13	Heterobimetallic Complexes That Bond Vanadium to Iron, Cobalt, and Nickel. Inorganic Chemistry, 2015, 54, 11669-11679.	4.0	45
14	Can Multiconfigurational Self-Consistent Field Theory and Density Functional Theory Correctly Predict the Ground State of Metalâ€“Metal-Bonded Complexes?. Journal of Chemical Theory and Computation, 2015, 11, 4093-4101.	5.3	20
15	Pushing the Limits of Delta Bonding in Metalâ€“Chromium Complexes with Redox Changes and Metal Swapping. Inorganic Chemistry, 2015, 54, 7579-7592.	4.0	46
16	Multiconfiguration Pair-Density Functional Theory: A Fully Translated Gradient Approximation and Its Performance for Transition Metal Dimers and the Spectroscopy of Re₂Cl₈^{2â€“}. Journal of Chemical Theory and Computation, 2015, 11, 4077-4085.	5.3	91
17	Bimetallic Cobaltâ€“Dinitrogen Complexes: Impact of the Supporting Metal on N₂ Activation. Inorganic Chemistry, 2015, 54, 9263-9270.	4.0	77
18	Free-radical copolymerisation of acrylamides, acrylates, and Î±-olefins. Molecular Physics, 2015, 113, 1809-1822.	1.7	2

#	Article	IF	Citations
19	Influence of Copper Oxidation State on the Bonding and Electronic Structure of Cobaltâ€“Copper Complexes. Inorganic Chemistry, 2015, 54, 11330-11338.	4.0	12
20	Multiconfiguration Pair-Density Functional Theory: Barrier Heights and Main Group and Transition Metal Energetics. Journal of Chemical Theory and Computation, 2015, 11, 82-90.	5.3	62
21	Synthesis and redox reactivity of a phosphine-ligated dichromium paddlewheel. Inorganica Chimica Acta, 2015, 424, 336-344.	2.4	4
22	Role of the Metal in the Bonding and Properties of Bimetallic Complexes Involving Manganese, Iron, and Cobalt. Journal of the American Chemical Society, 2014, 136, 1842-1855.	13.7	91
23	Predicting paramagnetic ¹H NMR chemical shifts and state-energy separations in spin-crossover hostâ€“guest systems. Physical Chemistry Chemical Physics, 2014, 16, 10620-10628.	2.8	32
24	Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 3669-3680.	5.3	334