

# Rebecca K Carlson

## List of Publications by Year in descending order

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Version: 2024-02-01

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	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	3.3	1,317
2	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	5.3	661
3	Multiconfiguration Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3669-3680.	5.3	334
4	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. <i>Accounts of Chemical Research</i> , 2017, 50, 66-73.	15.6	232
5	Role of the Metal in the Bonding and Properties of Bimetallic Complexes Involving Manganese, Iron, and Cobalt. <i>Journal of the American Chemical Society</i> , 2014, 136, 1842-1855.	13.7	91
6	Multiconfiguration Pair-Density Functional Theory: A Fully Translated Gradient Approximation and Its Performance for Transition Metal Dimers and the Spectroscopy of $\text{Re}_2\text{Cl}_8^{2+}$ . <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4077-4085.	5.3	91
7	Computationally Guided Discovery of a Catalytic Cobalt-Decorated Metal-Organic Framework for Ethylene Dimerization. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23576-23583.	3.1	78
8	Bimetallic Cobalt-Dinitrogen Complexes: Impact of the Supporting Metal on $\text{N}_2$ Activation. <i>Inorganic Chemistry</i> , 2015, 54, 9263-9270.	4.0	77
9	Multiconfiguration Pair-Density Functional Theory: Barrier Heights and Main Group and Transition Metal Energetics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 82-90.	5.3	62
10	Separated-pair approximation and separated-pair pair-density functional theory. <i>Chemical Science</i> , 2016, 7, 2399-2413.	7.4	47
11	Pushing the Limits of Delta Bonding in Metal-Chromium Complexes with Redox Changes and Metal Swapping. <i>Inorganic Chemistry</i> , 2015, 54, 7579-7592.	4.0	46
12	Heterobimetallic Complexes That Bond Vanadium to Iron, Cobalt, and Nickel. <i>Inorganic Chemistry</i> , 2015, 54, 11669-11679.	4.0	45
13	Predicting paramagnetic $^1\text{H}$ NMR chemical shifts and state-energy separations in spin-crossover host-guest systems. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10620-10628.	2.8	32
14	Structure and bonding of group 4-nickel heterobimetallics supported by 2-(diphenylphosphino)pyrrolide ligands. <i>Dalton Transactions</i> , 2016, 45, 9892-9901.	3.3	24
15	Can Multiconfigurational Self-Consistent Field Theory and Density Functional Theory Correctly Predict the Ground State of Metal-Metal-Bonded Complexes?. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4093-4101.	5.3	20
16	On-Top Pair Density as a Measure of Left-Right Correlation in Bond Breaking. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5540-5547.	2.5	13
17	Influence of Copper Oxidation State on the Bonding and Electronic Structure of Cobalt-Copper Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 11330-11338.	4.0	12
18	Spectroscopic and electrochemical characterization of a $\text{Pr}^{4+}$ imidophosphorane complex and the redox chemistry of $\text{Nd}^{3+}$ and $\text{Dy}^{3+}$ complexes. <i>Dalton Transactions</i> , 2022, 51, 6696-6706.	3.3	11

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19	Synthesis and characterization of triply-bonded titanium-iron complexes supported by 2-(diphenylphosphino)pyrrolide ligands. <i>Inorganica Chimica Acta</i> , 2017, 460, 43-48.	2.4	10
20	Tight-Binding Modeling of Uranium in an Aqueous Environment. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3073-3083.	5.3	6
21	Synthesis and redox reactivity of a phosphine-ligated dichromium paddlewheel. <i>Inorganica Chimica Acta</i> , 2015, 424, 336-344.	2.4	4
22	Free-radical copolymerisation of acrylamides, acrylates, and $\hat{1}\pm$ -olefins. <i>Molecular Physics</i> , 2015, 113, 1809-1822.	1.7	2
23	On-Top Ratio for Atoms and Molecules. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8294-8304.	2.5	2
24	Mechanistic Study of the Production of NO <sub>x</sub> Gases from the Reaction of Copper with Nitric Acid. <i>Inorganic Chemistry</i> , 2020, 59, 16833-16842.	4.0	1