Rebecca K Carlson

List of Publications by Citations

24 papers	2,333 citations	15 h-index	30 g-index
30 ext. papers	2,825 ext. citations	5.9 avg, IF	4.42 L-index

#	Paper	IF	Citations
24	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
23	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
22	Multiconfiguration Pair-Density Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 3669-80	6.4	246
21	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. *Accounts of Chemical Research*, **2017**, 50, 66-73	24.3	175
20	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, 1842-55	16.4	78
19	Multiconfiguration Pair-Density Functional Theory: A Fully Translated Gradient Approximation and Its Performance for Transition Metal Dimers and the Spectroscopy of Re2Cl8(2-). *Journal of Chemical Theory and Computation*, **2015**, 11, 4077-85	6.4	67
18	Computationally Guided Discovery of a Catalytic Cobalt-Decorated Metal–Organic Framework for Ethylene Dimerization. *Journal of Physical Chemistry C*, **2016**, 120, 23576-23583	3.8	67
17	Bimetallic cobalt-dinitrogen complexes: impact of the supporting metal on N2 activation. *Inorganic Chemistry*, **2015**, 54, 9263-70	5.1	63
16	Multiconfiguration pair-density functional theory: barrier heights and main group and transition metal energetics. *Journal of Chemical Theory and Computation*, **2015**, 11, 82-90	6.4	44
15	Pushing the Limits of Delta Bonding in Metal-Chromium Complexes with Redox Changes and Metal Swapping. *Inorganic Chemistry*, **2015**, 54, 7579-92	5.1	38
14	Separated-pair approximation and separated-pair pair-density functional theory. *Chemical Science*, **2016**, 7, 2399-2413	9.4	37
13	Heterobimetallic Complexes That Bond Vanadium to Iron, Cobalt, and Nickel. *Inorganic Chemistry*, **2015**, 54, 11669-79	5.1	37
12	Predicting paramagnetic 1H NMR chemical shifts and state-energy separations in spin-crossover host-guest systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 10620-8	3.6	31
11	Structure and bonding of group 4-nickel heterobimetallics supported by 2-(diphenylphosphino)pyrrolide ligands. *Dalton Transactions*, **2016**, 45, 9892-901	4.3	21
10	Can Multiconfigurational Self-Consistent Field Theory and Density Functional Theory Correctly Predict the Ground State of Metal-Metal-Bonded Complexes?. *Journal of Chemical Theory and Computation*, **2015**, 11, 4093-101	6.4	16
9	Influence of Copper Oxidation State on the Bonding and Electronic Structure of Cobalt-Copper Complexes. *Inorganic Chemistry*, **2015**, 54, 11330-8	5.1	12
8	On-Top Pair Density as a Measure of Left-Right Correlation in Bond Breaking. *Journal of Physical Chemistry A*, **2017**, 121, 5540-5547	2.8	12

List of Publications

7	Synthesis and characterization of triply-bonded titanium-iron complexes supported by 2-(diphenylphosphino)pyrrolide ligands. *Inorganica Chimica Acta*, **2017**, 460, 43-48	2.7	9
6	Synthesis and redox reactivity of a phosphine-ligated dichromium paddlewheel. *Inorganica Chimica Acta*, **2015**, 424, 336-344	2.7	4
5	OpenMolcas: From Source Code to Insight		4
4	On-Top Ratio for Atoms and Molecules. *Journal of Physical Chemistry A*, **2019**, 123, 8294-8304	2.8	2
3	Free-radical copolymerisation of acrylamides, acrylates, and olefins. *Molecular Physics*, **2015**, 113, 1809-1822	1.7	2
2	Tight-Binding Modeling of Uranium in an Aqueous Environment. *Journal of Chemical Theory and Computation*, **2020**, 16, 3073-3083	6.4	2
1	Mechanistic Study of the Production of NO Gases from the Reaction of Copper with Nitric Acid. *Inorganic Chemistry*, **2020**, 59, 16833-16842	5.1	1