

# Christine M Morales

## List of Publications by Year in descending order

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13  
papers

387  
citations

1040056

9  
h-index

1125743

13  
g-index

13  
all docs

13  
docs citations

13  
times ranked

571  
citing authors

#	ARTICLE	IF	CITATIONS
1	$\Delta$ SCF calculations of core electron binding energies in first-row transition metal atoms. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	2.0	4
2	Exploration of Substituent and Isotope Effects on Reaction Rates by a Computational Modeling Experiment. <i>Journal of Chemical Education</i> , 2019, 96, 792-796.	2.3	1
3	Molecular-Level Mechanisms of Vibrational Frequency Shifts in a Polar Liquid. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7597-7605.	2.6	18
4	Supramolecular main-chain liquid crystalline polymers and networks with competitive hydrogen bonding. <i>Liquid Crystals</i> , 2010, 37, 1127-1131.	2.2	13
5	Electronic Structural Comparison of the Reactions of Dioxygen and Alkenes with Nitrogen-Chelated Palladium(0). <i>Inorganic Chemistry</i> , 2010, 49, 8200-8207.	4.0	23
6	Simulations of Infrared Spectra of Nanoconfined Liquids: Acetonitrile Confined in Nanoscale, Hydrophilic Silica Pores. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1922-1933.	2.5	64
7	Umbrella Sampling of Solute Vibrational Line Shifts in Mixed Quantum-Classical Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2008, 112, 313-320.	2.6	2
8	Mixed Quantum-Classical Molecular Dynamics Analysis of the Molecular-Level Mechanisms of Vibrational Frequency Shifts. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5422-5433.	2.5	5
9	Computational Studies of Metal-Ligand Bond Enthalpies across the Transition Metal Series. <i>Organometallics</i> , 2006, 25, 5566-5581.	2.3	62
10	Catalytic hydroxylation of 1-propanol by platinum NCN and PCP pincer complexes using CuCl <sub>2</sub> as oxidant. <i>Inorganica Chimica Acta</i> , 2006, 359, 1923-1928.	2.4	36
11	Characterization of titanium dopants in sodium alanate by electron paramagnetic resonance spectroscopy. <i>Journal of Materials Research</i> , 2005, 20, 3265-3269.	2.6	15
12	Inverse-Electron-Demand Ligand Substitution: Experimental and Computational Insights into Olefin Exchange at Palladium(0). <i>Journal of the American Chemical Society</i> , 2004, 126, 14832-14842.	13.7	41
13	Insights into the Spin-Forbidden Reaction between L <sub>2</sub> Pd <sup>0</sup> and Molecular Oxygen. <i>Journal of the American Chemical Society</i> , 2004, 126, 16302-16303.	13.7	103