Christine M Morales

List of Publications by Year
in descending order

13	387	1040056 9	1125743 13
papers	citations	h-index	g-index

13	13	13	571
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Insights into the Spin-Forbidden Reaction between L2Pd0 and Molecular Oxygen. Journal of the American Chemical Society, 2004, 126, 16302-16303.	13.7	103
2	Simulations of Infrared Spectra of Nanoconfined Liquids: Acetonitrile Confined in Nanoscale, Hydrophilic Silica Pores. Journal of Physical Chemistry A, 2009, 113, 1922-1933.	2.5	64
3	Computational Studies of Metalâ˜Ligand Bond Enthalpies across the Transition Metal Series. Organometallics, 2006, 25, 5566-5581.	2.3	62
4	â€œInverse-Electron-Demandâ€•Ligand Substitution:Â Experimental and Computational Insights into Olefin Exchange at Palladium(0). Journal of the American Chemical Society, 2004, 126, 14832-14842.	13.7	41
5	Catalytic hydroxylation of 1-propanol by platinum NCN and PCP pincer complexes using CuCl2 as oxidant. Inorganica Chimica Acta, 2006, 359, 1923-1928.	2.4	36
6	Electronic Structural Comparison of the Reactions of Dioxygen and Alkenes with Nitrogen-Chelated Palladium(0). Inorganic Chemistry, 2010, 49, 8200-8207.	4.0	23
7	Molecular-Level Mechanisms of Vibrational Frequency Shifts in a Polar Liquid. Journal of Physical Chemistry B, 2011, 115, 7597-7605.	2.6	18
8	Characterization of titanium dopants in sodium alanate by electron paramagnetic resonance spectroscopy. Journal of Materials Research, 2005, 20, 3265-3269.	2.6	15
9	Supramolecular main-chain liquid crystalline polymers and networks with competitive hydrogen bonding. Liquid Crystals, 2010, 37, 1127-1131.	2.2	13
10	Mixed Quantum-Classical Molecular Dynamics Analysis of the Molecular-Level Mechanisms of Vibrational Frequency Shifts. Journal of Physical Chemistry A, 2007, 111, 5422-5433.	2.5	5
11	<scp>Î”â€ŠSCF</scp> calculations of core electron binding energies in firstâ€row transition metal atoms. International Journal of Quantum Chemistry, 2022, 122, .	2.0	4
12	Umbrella Sampling of Solute Vibrational Line Shifts in Mixed Quantumâ˜Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 313-320.	2.6	2
13	Exploration of Substituent and Isotope Effects on Reaction Rates by a Computational Modeling Experiment. Journal of Chemical Education, 2019, 96, 792-796.	2.3	1