Christoph Loschen

List of Publications by Year
in descending order

23	1,207	471509 17	642732 23
papers	citations	h-index	g-index

26	26	26	1642
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Rational Coformer or Solvent Selection for Pharmaceutical Cocrystallization or Desolvation. Journal of Pharmaceutical Sciences, 2012, 101, 3687-3697.	3.3	150
2	Density functional studies of model cerium oxide nanoparticles. Physical Chemistry Chemical Physics, 2008, 10, 5730.	2.8	125
3	Electronic structure of COâ€"An exercise in modern chemical bonding theory. Journal of Computational Chemistry, 2007, 28, 117-126.	3.3	114
4	Solubility prediction, solvate and cocrystal screening as tools for rational crystal engineering. Journal of Pharmacy and Pharmacology, 2015, 67, 803-811.	2.4	102
5	Understanding Ceria Nanoparticles from First-Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 10142-10145.	3.1	99
6	Edge sites as a gate for subsurface carbon in palladium nanoparticles. Journal of Catalysis, 2009, 266, 59-63.	6.2	71
7	Prediction of Solubilities and Partition Coefficients in Polymers Using COSMO-RS. Industrial & Engineering Chemistry Research, 2014, 53, 11478-11487.	3.7	62
8	Extending the NHC Concept: C-C Coupling Catalysis by a PdII Carbene (rNHC) Complex with Remote Heteroatoms. European Journal of Inorganic Chemistry, 2005, 2005, 2973-2977.	2.0	59
9	Why Are Olefins Oxidized by RuO4under Cleavage of the Carbonâ^'Carbon Bond whereas Oxidation by OsO4Yieldscis-Diols?â€. Journal of the American Chemical Society, 2004, 126, 3642-3652.	13.7	58
10	COSMOquick: A Novel Interface for Fast Ïƒ-Profile Composition and Its Application to COSMO-RS Solvent Screening Using Multiple Reference Solvents. Industrial & Engineering Chemistry Research, 2012, 51, 14303-14308.	3.7	50
11	Atomic and Electronic Structure of Cerium Oxide Stepped Model Surfaces. Journal of Physical Chemistry C, 2008, 112, 17643-17651.	3.1	40
12	Quantum Chemical Investigations and Bonding Analysis of Iron Complexes with Mixed Cyano and Carbonyl Ligands. Inorganic Chemistry, 2004, 43, 778-784.	4.0	37
13	Performance of planeâ€waveâ€based LDA+U and GGA+U approaches to describe magnetic coupling in molecular systems. Journal of Computational Chemistry, 2009, 30, 2316-2326.	3.3	35
14	Computational Screening of Drug Solvates. Pharmaceutical Research, 2016, 33, 2794-2804.	3.5	32
15	Towards size-converged properties of model ceria nanoparticles: Monitoring by adsorbed CO using DFT +U approach. Chemical Physics Letters, 2008, 465, 106-109.	2.6	31
16	COSMO-RS based predictions for the SAMPL6 logP challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 385-392.	2.9	30
17	Cocrystal Ternary Phase Diagrams from Density Functional Theory and Solvation Thermodynamics. Crystal Growth and Design, 2018, 18, 5600-5608.	3.0	21
18	Theoretical studies of ethylene addition to transition metal compounds with carbene and oxo groups LnM(ï£¾CH2)(ï£¾O). Journal of Physical Organic Chemistry, 2007, 20, 11-18.	1.9	18

#	Article	IF	Citations
19	Synthesis, Structure and Reactivity of Trimethylsilyl-Substituted Phosphametallocenes. European Journal of Inorganic Chemistry, 2007, 2007, 553-561.	2.0	17
20	Reaction of Tungsten Î·1-Acetylide Complexes [(Î·5-C5H5)(NO)(CO)Wâ^'Câ‹®Câ^'R]Li with Iminium Ions. Organometallics, 2005, 24, 977-989.	2.3	16
21	Ethylene addition to OsO3(CH2) â€“ A theoretical study. Journal of Organometallic Chemistry, 2006, 691, 4467-4473.	1.8	13
22	The nature of the metalâ€“nitric oxide bond in the [M(CN)5(NO)]q (M=Cr, Mn, Fe, Ru, Os, and Co) and trans-[Ru(NH3)4L(NO)]q (L=pyrazine, pyridine, N2, H2O, Clâ^', CNâ^',) complexes: A bond-energy decomposition analysis. Computational and Theoretical Chemistry, 2008, 865, 28-35.	1.5	13
23	Ab Initio Kinetic Modeling of Living Anionic and Zwitterionic Chain Polymerization Mechanisms. Macromolecules, 2010, 43, 9674-9681.	4.8	9