

Christoph Loschen

List of Publications by Year in descending order

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23
papers

1,207
citations

471509

17
h-index

642732

23
g-index

26
all docs

26
docs citations

26
times ranked

1642
citing authors

#	ARTICLE	IF	CITATIONS
1	COSMO-RS based predictions for the SAMPL6 logP challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 385-392.	2.9	30
2	Cocrystal Ternary Phase Diagrams from Density Functional Theory and Solvation Thermodynamics. <i>Crystal Growth and Design</i> , 2018, 18, 5600-5608.	3.0	21
3	Computational Screening of Drug Solvates. <i>Pharmaceutical Research</i> , 2016, 33, 2794-2804.	3.5	32
4	Solubility prediction, solvate and cocrystal screening as tools for rational crystal engineering. <i>Journal of Pharmacy and Pharmacology</i> , 2015, 67, 803-811.	2.4	102
5	Prediction of Solubilities and Partition Coefficients in Polymers Using COSMO-RS. <i>Industrial & Engineering Chemistry Research</i> , 2014, 53, 11478-11487.	3.7	62
6	COSMO-quick: A Novel Interface for Fast Δf -Profile Composition and Its Application to COSMO-RS Solvent Screening Using Multiple Reference Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2012, 51, 14303-14308.	3.7	50
7	Rational Coformer or Solvent Selection for Pharmaceutical Cocrystallization or Desolvation. <i>Journal of Pharmaceutical Sciences</i> , 2012, 101, 3687-3697.	3.3	150
8	Ab Initio Kinetic Modeling of Living Anionic and Zwitterionic Chain Polymerization Mechanisms. <i>Macromolecules</i> , 2010, 43, 9674-9681.	4.8	9
9	Edge sites as a gate for subsurface carbon in palladium nanoparticles. <i>Journal of Catalysis</i> , 2009, 266, 59-63.	6.2	71
10	Performance of plane-wave based LDA+ U and GGA+ U approaches to describe magnetic coupling in molecular systems. <i>Journal of Computational Chemistry</i> , 2009, 30, 2316-2326.	3.3	35
11	Towards size-converged properties of model ceria nanoparticles: Monitoring by adsorbed CO using DFT+ U approach. <i>Chemical Physics Letters</i> , 2008, 465, 106-109.	2.6	31
12	The nature of the metal-nitric oxide bond in the $[M(CN)_5(NO)]_q$ ($M=Cr, Mn, Fe, Ru, Os, \text{ and } Co$) and $trans-[Ru(NH_3)_4L(NO)]_q$ ($L=pyrazine, pyridine, N_2, H_2O, Cl^-, CN^-,$) complexes: A bond-energy decomposition analysis. <i>Computational and Theoretical Chemistry</i> , 2008, 865, 28-35.	1.5	13
13	Density functional studies of model cerium oxide nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5730.	2.8	125
14	Atomic and Electronic Structure of Cerium Oxide Stepped Model Surfaces. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17643-17651.	3.1	40
15	Understanding Ceria Nanoparticles from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 10142-10145.	3.1	99
16	Electronic structure of CO: An exercise in modern chemical bonding theory. <i>Journal of Computational Chemistry</i> , 2007, 28, 117-126.	3.3	114
17	Synthesis, Structure and Reactivity of Trimethylsilyl-Substituted Phosphametalloenes. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 553-561.	2.0	17
18	Theoretical studies of ethylene addition to transition metal compounds with carbene and oxo groups $LnM(\frac{3}{4}CH_2)(\frac{3}{4}O)$. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 11-18.	1.9	18

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19	Ethylene addition to OsO ₃ (CH ₂) – A theoretical study. Journal of Organometallic Chemistry, 2006, 691, 4467-4473.	1.8	13
20	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
21	Reaction of Tungsten η^5 -Acetylide Complexes [(η^5 -C ₅ H ₅)(NO)(CO)W ⁺ C ₂ R]Li with Iminium Ions. Organometallics, 2005, 24, 977-989.	2.3	16
22	Why Are Olefins Oxidized by RuO ₄ under Cleavage of the Carbon-Carbon Bond whereas Oxidation by OsO ₄ Yields cis-Diols? Journal of the American Chemical Society, 2004, 126, 3642-3652.	13.7	58
23	Quantum Chemical Investigations and Bonding Analysis of Iron Complexes with Mixed Cyano and Carbonyl Ligands. Inorganic Chemistry, 2004, 43, 778-784.	4.0	37