

Patrick Jacques Merkling

List of Publications by Year in descending order

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Version: 2024-02-01

23
papers

815
citations

567281

15
h-index

642732

23
g-index

23
all docs

23
docs citations

23
times ranked

1328
citing authors

#	ARTICLE	IF	CITATIONS
1	The hydration of Cu ²⁺ : Can the Jahn-Teller effect be detected in liquid solution?. Journal of Chemical Physics, 2006, 124, 064509.	3.0	104
2	Ab initio x-ray absorption study of copper K-edge XANES spectra in Cu(II) compounds. Physical Review B, 2005, 71, .	3.2	82
3	Low-coverage adsorption properties of the metal-organic framework MIL-47 studied by pulse chromatography and Monte Carlo simulations. Physical Chemistry Chemical Physics, 2009, 11, 3515.	2.8	73
4	Exploring the Capabilities of X-ray Absorption Spectroscopy for Determining the Structure of Electrolyte Solutions: Computed Spectra for Cr ³⁺ or Rh ³⁺ in Water Based on Molecular Dynamics. Journal of the American Chemical Society, 2002, 124, 10911-10920.	13.7	72
5	Nature of Metal Binding Sites in Cu(II) Complexes with Histidine and Related N-Coordinating Ligands, As Studied by EXAFS. Inorganic Chemistry, 2004, 43, 6674-6683.	4.0	61
6	Enantioselective adsorption of ibuprofen and lysine in metal-organic frameworks. Chemical Communications, 2014, 50, 10849.	4.1	52
7	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. Chemistry of Materials, 2015, 27, 5657-5667.	6.7	42
8	Combination of XANES spectroscopy and molecular dynamics to probe the local structure in disordered systems. Physical Review B, 2001, 64, .	3.2	38
9	Molecular Sieves for the Separation of Hydrogen Isotopes. ACS Applied Materials & Interfaces, 2019, 11, 18833-18840.	8.0	36
10	Interplay of computer simulations and x-ray absorption spectra in the study of the bromide hydration structure. Journal of Chemical Physics, 2003, 119, 6647-6654.	3.0	33
11	Zeolites for CO ₂ Separation to Obtain CO ₂ -Neutral Fuels. ACS Applied Materials & Interfaces, 2018, 10, 20512-20520.	8.0	30
12	Spectroscopic Investigation of the Gas-Phase Conformations of 15-Crown-5 Ether Complexes with K ⁺ . Journal of Physical Chemistry A, 2009, 113, 7748-7752.	2.5	29
13	Molecular-dynamics-based investigation of scattering path contributions to the EXAFS spectrum: The Cr ³⁺ aqueous solution case. Physical Review B, 2001, 64, .	3.2	28
14	Synthesis and Characterization of Elongated-Shaped Silver Nanoparticles as a Biocompatible Anisotropic SERS Probe for Intracellular Imaging: Theoretical Modeling and Experimental Verification. Nanomaterials, 2019, 9, 256.	4.1	27
15	N ² -(Azol-1(2)-yl)ethyliminodiacetic acids: a novel series of Gd(III) chelators as T ₂ relaxation agents for magnetic resonance imaging. Bioorganic and Medicinal Chemistry, 1999, 7, 517-527.	3.0	22
16	Vapour-liquid equilibrium of fluids composed by oblate molecules. Molecular Physics, 2008, 106, 1331-1339.	1.7	14
17	A Simulation Study of Hydrogen in Metal-Organic Frameworks. Adsorption Science and Technology, 2010, 28, 823-835.	3.2	14
18	Influence of Flexibility on the Separation of Chiral Isomers in STW-type Zeolite. Chemistry - A European Journal, 2018, 24, 4121-4132.	3.3	14

#	ARTICLE	IF	CITATIONS
19	Impact of Small Adsorbates in the Vibrational Spectra of Mg- and Zn-MOF-74 Revealed by First-Principles Calculations. ACS Applied Materials & Interfaces, 2020, 12, 54980-54990.	8.0	14
20	Cadmium- ^{II} -BINOL Metal-Organic Framework for the Separation of Alcohol Isomers. Chemistry - A European Journal, 2017, 23, 874-885.	3.3	12
21	Separation of Amyl Alcohol Isomers in ZIF-77. ChemPhysChem, 2015, 16, 2735-2738.	2.1	8
22	Diffusion Patterns in Zeolite MFI: The Cation Effect. Journal of Physical Chemistry C, 2018, 122, 29274-29284.	3.1	6
23	EGFR-targeting antitumor therapy: Neuregulins or antibodies?. European Journal of Pharmaceutical Sciences, 2021, 158, 105678.	4.0	4