PaweÅ, Kozyra

List of Publications by Year
in descending order

17	209	1163117 8	1058476 14
papers	citations	h-index	g-index

17	17	17	198
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Water adsorption in ideal and defective UiO-66 structures. Microporous and Mesoporous Materials, 2022, 330, 111555.	4.4	28
2	Effect of Synthesis Temperature on Water Adsorption in UiO-66 Derivatives: Experiment, DFT+D Modeling, and Monte Carlo Simulations. Journal of Physical Chemistry C, 2022, 126, 9185-9194.	3.1	6
3	Zeolites at the Molecular Level: What Can Be Learned from Molecular Modeling. Molecules, 2021, 26, 1511.	3.8	6
4	Toward the Mechanism of o-Xylene Isomerization in Selected Zeolites of Different Si/Al Ratios and Channel Sizesâ€"Experiment Corroborated by Periodic DFT + D Simulations. Journal of Physical Chemistry C, 2021, 125, 10334-10348.	3.1	4
5	Trojan Horse Thiocyanate: Induction and Control of High Proton Conductivity in CPO-27/MOF-74 Metalâ€"Organic Frameworks by Metal Selection and Solvent-Free Mechanochemical Dosing. ACS Applied Materials & Interfaces, 2021, 13, 29820-29826.	8.0	5
6	Structural Studies of Aluminated form of Zeolitesâ€"EXAFS and XRD Experiment, STEM Micrography, and DFT Modelling. Molecules, 2021, 26, 3566.	3.8	2
7	Carbon Dioxide Capture Enhanced by Preâ€Adsorption of Water and Methanol in UiOâ€66. Chemistry - A European Journal, 2021, 27, 14653-14659.	3.3	17
8	A comparative computational study on hydrogen adsorption on the Ag⁺, Cu⁺, Mg²⁺, Cd²⁺, and Zn²⁺ cationic sites in zeolites. Physical Chemistry Chemical Physics, 2016, 18, 12592-12603.	2.8	19
9	Spin-resolved NOCV analysis of the zeolite framework influence on the interaction of NO with Cu(<scp>i</scp>/<scp>ii</scp>) sites in zeolites. Physical Chemistry Chemical Physics, 2015, 17, 13267-13273.	2.8	2
10	Extinction coefficients of CC and CC bands in ethyne and ethene molecules interacting with Cu+ and Ag+ in zeolites â€" IR studies and quantumchemical DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1988-1992.	3.9	4
11	Electronic propensity of Cu(II) versus Cu(I) sites in zeolites to activate NO â€" Spin- and orbital-resolved Cuâ€"NO electron transfer. Canadian Journal of Chemistry, 2013, 91, 538-543.	1.1	9
12	Câ•€, Câ‰¡C, and Câ•Ð Bond Activation by Coinage Metal Cations in ZSM-5 Zeolites: Quantitative Charge Transfer Resolution. Journal of Physical Chemistry C, 2013, 117, 7511-7518.	3.1	16
13	Ag+ and Cu+ Cations Ligated by Zeolite Environment Enhancing Hydrogen Activation â^' ETS-NOCV Charge-Transfer Analysis. Journal of Computer Chemistry Japan, 2013, 12, 30-37.	0.1	2
14	Cobalt cationic sites in ferrierites: QM/MM modeling. Catalysis Today, 2008, 137, 493-497.	4.4	7
15	The interaction of benzene with Cu+ sites in zeolites. Applied Catalysis A: General, 2006, 307, 46-50.	4.3	23
16	TPDâ€"IR studies of CO desorption from zeolites CuY and CuX. Journal of Molecular Structure, 2005, 744-747, 991-996.	3.6	30
17	IR studies and DFT quantum chemical calculations concerning interaction of some organic molecules with Cu+ sites in zeolites. Comptes Rendus Chimie, 2005, 8, 491-508.	0.5	29