Kaido Sillar

List of Publications by Year
in descending order

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15 papers	765 citations	687363 13 h-index	996975 15 g-index
15 all docs	15 docs citations	15 times ranked	1120 citing authors

#	Article	IF	Citations
1	Predicting adsorption selectivities from pure gas isotherms for gas mixtures in metalâ€“organic frameworks. Chemical Science, 2020, 11, 643-655.	7.4	19
2	Ab Initio Prediction of Adsorption Isotherms for Gas Mixtures by Grand Canonical Monte Carlo Simulations on a Lattice of Sites. Journal of Physical Chemistry Letters, 2017, 8, 2713-2718.	4.6	21
3	Ab Initio Adsorption Isotherms for Molecules with Lateral Interactions: CO₂ in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 12789-12799.	3.1	33
4	Ab Initio Prediction of Adsorption Isotherms for Small Molecules in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 14047-14056.	13.7	62
5	Hydrogen adsorbed in a metal organic framework-5: Coupled translation-rotation eigenstates from quantum five-dimensional calculations. Journal of Chemical Physics, 2012, 137, 014701.	3.0	43
6	Ab Initio Prediction of Adsorption Isotherms for Small Molecules in Metalâ€“Organic Frameworks: The Effect of Lateral Interactions for Methane/CPO-27-Mg. Journal of the American Chemical Society, 2012, 134, 18354-18365.	13.7	90
7	Heats of Adsorption of CO and CO₂ in Metalâ€“Organic Frameworks: Quantum Mechanical Study of CPO-27-M (M = Mg, Ni, Zn). Journal of Physical Chemistry C, 2011, 115, 21777-21784.	3.1	122
8	Computational Study of Cesium Cation Interactions with Neutral and Anionic Compounds Related to Soil Organic Matter. Journal of Physical Chemistry A, 2009, 113, 10734-10744.	2.5	19
9	Ab Initio Study of Hydrogen Adsorption in MOF-5. Journal of the American Chemical Society, 2009, 131, 4143-4150.	13.7	225
10	Adsorption of carbon monoxide on Li-ZSM-5: theoretical study of complexation of Li+ cation with two CO molecules. Physical Chemistry Chemical Physics, 2007, 9, 824.	2.8	10
11	Computational study of vibrational frequencies of bridging hydroxyl groups in zeolite ZSM-5. Chemical Physics Letters, 2004, 393, 285-289.	2.6	16
12	Hybrid Quantum Chemical and Density Functional Theory (ONIOM) Study of the Acid Sites in Zeolite ZSM-5. Journal of Physical Chemistry B, 2004, 108, 9893-9899.	2.6	52
13	Calculation of the properties of acid sites of the zeolite ZSM-5 using ONIOM method. Computational and Theoretical Chemistry, 2002, 589-590, 281-290.	1.5	27
14	Acidity of saturated hydrocarbons. Computational and Theoretical Chemistry, 2001, 535, 49-59.	1.5	8
15	Gas-phase basicities and proton affinities of alkali metal oxides and hydroxides. A theoretical study. Computational and Theoretical Chemistry, 2001, 543, 223-231.	1.5	18