LukÃ¡Å¡ Grajciar

List of Publications by Year
in descending order

33 papers	1,877 citations	331670 21 h-index	434195 31 g-index
35 all docs	35 docs citations	35 times ranked	2493 citing authors

#	Article	IF	Citations
1	A family of zeolites with controlled pore size prepared using a top-down method. Nature Chemistry, 2013, 5, 628-633.	13.6	355
2	Towards operando computational modeling in heterogeneous catalysis. Chemical Society Reviews, 2018, 47, 8307-8348.	38.1	169
3	Water Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. Journal of Physical Chemistry Letters, 2010, 1, 3354-3359.	4.6	166
4	Understanding CO₂ Adsorption in CuBTC MOF: Comparing Combined DFTâ€“ab Initio Calculations with Microcalorimetry Experiments. Journal of Physical Chemistry C, 2011, 115, 17925-17933.	3.1	146
5	Controlling the Adsorption Enthalpy of CO₂ in Zeolites by Framework Topology and Composition. ChemSusChem, 2012, 5, 2011-2022.	6.8	93
6	Accurate Prediction of Methane Adsorption in a Metalâ€“Organic Framework with Unsaturated Metal Sites by Direct Implementation of an ab Initio Derived Potential Energy Surface in GCMC Simulation. Journal of Physical Chemistry C, 2011, 115, 23074-23080.	3.1	86
7	Adsorption of CO2 in FAU zeolites: Effect of zeolite composition. Catalysis Today, 2014, 227, 50-56.	4.4	80
8	Fast room temperature lability of aluminosilicate zeolites. Nature Communications, 2019, 10, 4690.	12.8	75
9	Zeolite (In)Stability under Aqueous or Steaming Conditions. Advanced Materials, 2020, 32, e2003264.	21.0	75
10	Computational and FTIR spectroscopic studies on carbon monoxide and dinitrogen adsorption on a high-silica H-FER zeolite. Physical Chemistry Chemical Physics, 2009, 11, 791-802.	2.8	73
11	Accurate Description of Argon and Water Adsorption on Surfaces of Graphene-Based Carbon Allotropes. Journal of Physical Chemistry A, 2011, 115, 11387-11393.	2.5	68
12	Combined Theoretical and Experimental Investigation of CO Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. ChemPhysChem, 2012, 13, 488-495.	2.1	53
13	Periodic DFT investigation of the effect of aluminium content on the properties of the acid zeolite H-FER. Physical Chemistry Chemical Physics, 2010, 12, 1497.	2.8	49
14	Adsorption of Propane and Propylene on CuBTC Metalâ€“Organic Framework: Combined Theoretical and Experimental Investigation. Journal of Physical Chemistry C, 2013, 117, 11159-11167.	3.1	48
15	The effect of water on the validity of LÃ¶wenstein's rule. Chemical Science, 2019, 10, 5705-5711.	7.4	37
16	Accurate Ab Initio Description of Adsorption on Coordinatively Unsaturated Cu2+ and Fe3+ Sites in MOFs. Journal of Chemical Theory and Computation, 2015, 11, 230-238.	5.3	36
17	Theoretical investigation of layered zeolite frameworks: Interaction between IPC-1P layers derived from zeolite UTL. Catalysis Today, 2013, 204, 15-21.	4.4	33
18	Density functional theory for molecular and periodic systems using density fitting and continuous fast multipole method: Analytical gradients. Journal of Computational Chemistry, 2016, 37, 2518-2526.	3.3	29

#	Article	IF	Citations
19	Intrinsic valley polarization in 2D magnetic MXenes: surface engineering induced spin-valley coupling. Journal of Materials Chemistry C, 2021, 9, 11132-11141.	5.5	29
20	Control of CO2adsorption heats by the Al distribution in FER zeolites. Physical Chemistry Chemical Physics, 2012, 14, 1117-1120.	2.8	28
21	Control of spintronic and electronic properties of bimetallic and vacancy-ordered vanadium carbide MXenes via surface functionalization. Physical Chemistry Chemical Physics, 2019, 21, 25802-25808.	2.8	22
22	The BrÃ¸nsted acidity of three- and two-dimensional zeolites. Microporous and Mesoporous Materials, 2019, 282, 121-132.	4.4	21
23	Origin of the Unusual Stability of Zeolite-Encapsulated Sub-Nanometer Platinum. ACS Catalysis, 2020, 10, 11057-11068.	11.2	20
24	Lowâ€memory iterative density fitting. Journal of Computational Chemistry, 2015, 36, 1521-1535.	3.3	15
25	The Lewis acidity of three- and two-dimensional zeolites: The effect of framework topology. Catalysis Today, 2018, 304, 12-21.	4.4	13
26	PbS Clusters Embedded in Sodalite Zeolite Cavities of Different Compositions: Unraveling the Structural Evolution and Optical Properties Using ab Initio Calculations. Journal of Physical Chemistry C, 2016, 120, 27050-27065.	3.1	12
27	The Role of Water Loading and Germanium Content in Germanosilicate Hydrolysis. Journal of Physical Chemistry C, 2021, 125, 23744-23757.	3.1	12
28	Mechanism of Zeolite Hydrolysis under Basic Conditions. Chemistry of Materials, 2021, 33, 9202-9212.	6.7	9
29	Doping isolated one-dimensional antiferromagnetic semiconductor vanadium tetrasulfide (VS₄) nanowires with carriers induces half-metallicity. Journal of Materials Chemistry C, 2021, 9, 3122-3128.	5.5	8
30	Structure Determination of the Oxygen Evolution Catalyst MÃ¶ssbauerite. Journal of Physical Chemistry C, 2019, 123, 25157-25165.	3.1	7
31	Identification of the most active sites for tetrahydropyranylation in zeolites: MFI as a test case. Catalysis Today, 2020, 345, 165-174.	4.4	4
32	Accurate ab initio Description of Adsorption on Coordinatively Unsaturated Sites in Metalâ€“Organic Frameworks. , 2015, , 175-206.		3
33	Correction to Mechanism of Zeolite Hydrolysis under Basic Conditions. Chemistry of Materials, 0, , .	6.7	0