Lucyna Firlej

List of Publications by Year in descending order

42	981	567281 15	434195 31
papers	citations	h-index	g-index

43	43	43	1267
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High-throughput screening of metal â€“ Organic frameworks for CO2 and CH4 separation in the presence of water. Chemical Engineering Journal, 2021, 403, 126392.	12.7	53
2	Phonons and Adsorption-Induced Deformations in ZIFs: Is It Really a Gate Opening?. Journal of Physical Chemistry C, 2021, 125, 7999-8005.	3.1	10
3	Hydrogen Storage in Pure and Boron-Substituted Nanoporous Carbons-Numerical and Experimental Perspective. Nanomaterials, 2021, 11, .	4.1	0
4	Hydrogen Storage in Pure and Boron-Substituted Nanoporous Carbonsâ€"Numerical and Experimental Perspective. Nanomaterials, 2021, 11, 2173.	4.1	3
5	Effect of low frequency phonons on structural properties of ZIFs with SOD topology. Microporous and Mesoporous Materials, 2020, 304, 109132.	4.4	13
6	How dense is the gas adsorbed in nanopores?. Microporous and Mesoporous Materials, 2020, 304, 109240.	4.4	3
7	Acetone-derived luminescent polymer dots: a facile and low-cost synthesis leads to remarkable photophysical properties. RSC Advances, 2020, 10, 38437-38445.	3.6	7
8	Pore opening and breathing transitions in metal-organic frameworks: Coupling adsorption and deformation. Journal of Colloid and Interface Science, 2020, 578, 77-88.	9.4	20
9	Self-Assembled Two-Dimensional Nanoporous Crystals as Molecular Sieves: Molecular Dynamics Studies of 1,3,5-Tristyrilbenzene-Cn Superstructures. Journal of Chemical Information and Modeling, 2020, 60, 2155-2168.	5.4	3
10	Absorption of atomic and molecular species in carbon cellular structures (Review article). Low Temperature Physics, 2020, 46, 219-231.	0.6	5
11	Intermediate states approach for adsorption studies in flexible metalâ€"organic frameworks. Physical Chemistry Chemical Physics, 2019, 21, 3294-3303.	2.8	13
12	Phonons in deformable microporous crystalline solids. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 513-527.	0.8	7
13	Computer modeling of 2D supramolecular nanoporous monolayers self-assembled on graphite. Nanoscale, 2019, 11, 21284-21290.	5.6	2
14	Benchmarking of GGA density functionals for modeling structures of nanoporous, rigid and flexible MOFs. Journal of Chemical Physics, 2018, 149, 064110.	3.0	23
15	Modeling of low temperature adsorption of hydrogen in carbon nanopores. Journal of Molecular Modeling, 2017, 23, 20.	1.8	17
16	Evolution of methane density during melting in nanopores. Journal of Molecular Modeling, 2017, 23, 44.	1.8	2
17	Simulation and Characterization of Tetracosane on Graphite: Molecular Dynamics Beyond the Monolayer. Journal of Physical Chemistry C, 2016, 120, 984-994.	3.1	7
18	Hydrogen adsorption on surfaces with different binding energies. Chemical Data Collections, 2016, 2, 56-60.	2.3	3

#	Article	IF	Citations
19	Hydrogen storage by adsorption in porous materials: Is it possible?. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 496, 69-76.	4.7	32
20	Engineered Porous Carbon for High Volumetric Methane Storage. Adsorption Science and Technology, 2014, 32, 681-691.	3.2	16
21	Different Approach to Estimation of Hydrogen-Binding Energy in Nanospace-Engineered Activated Carbons. Journal of Physical Chemistry C, 2014, 118, 955-961.	3.1	7
22	Unique Bonding Nature of Carbon-Substituted Be₂ Dimer inside the Carbon (sp²) Network. Journal of Physical Chemistry A, 2014, 118, 5727-5733.	2.5	9
23	Open carbon frameworks - a search for optimal geometry for hydrogen storage. Journal of Molecular Modeling, 2013, 19, 4079-4087.	1.8	15
24	Understanding Universal Adsorption Limits for Hydrogen Storage in Nano Porous Systems. Advanced Materials, 2013, 25, 5971-5974.	21.0	28
25	Increased H2 gravimetric storage capacity in truncated carbon slit pores modeled by Grand Canonical Monte Carlo. Carbon, 2013, 53, 208-215.	10.3	18
26	Hypothetical High-Surface-Area Carbons with Exceptional Hydrogen Storage Capacities: Open Carbon Frameworks. Journal of the American Chemical Society, 2012, 134, 15130-15137.	13.7	66
27	Nanospace engineering of KOH activated carbon. Nanotechnology, 2012, 23, 015401.	2.6	301
28	Molecular simulations of intermediate and long alkanes adsorbed on graphite: Tuning of non-bond interactions. Journal of Molecular Modeling, 2011, 17, 811-816.	1.8	10
29	A review of boron enhanced nanoporous carbons for hydrogen adsorption: numerical perspective. Adsorption, 2010, 16, 413-421.	3.0	34
30	Influence of structural heterogeneity of nanoporous sorbent walls on hydrogen storage. Applied Surface Science, 2010, 256, 5270-5274.	6.1	14
31	Structural and energetic factors in designing a nanoporous sorbent for hydrogen storage. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2010, 357, 61-66.	4.7	27
32	Numerical estimation of hydrogen storage limits in carbon-based nanospaces. Carbon, 2010, 48, 223-231.	10.3	59
33	Molecular dynamics simulations of submonolayer hexane and pentane films on graphite. Molecular Simulation, 2010, 36, 326-333.	2.0	3
34	Enhanced hydrogen adsorption in boron substituted carbon nanospaces. Journal of Chemical Physics, 2009, 131, 164702.	3.0	50
35	Boron substituted graphene: energy landscape for hydrogen adsorption. Adsorption, 2009, 15, 312-317.	3.0	41
36	Melting of Hexane Monolayers Adsorbed on Graphite: The Role of Domains and Defect Formation. Langmuir, 2009, 25, 6596-6598.	3.5	13

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37	Influence of quantum effects on the mechanism of adsorption andÂphase diagram of rare gases in carbon nanotubes. Adsorption, 2008, 14, 719-726.	3.0	3
38	Influence of Strength of Atom-Wall Interactions on Adsorption Mechanism. Adsorption, 2005, 11, 367-372.	3.0	2
39	Monte Carlo simulations of krypton adsorption in nanopores: Influence of pore-wall heterogeneity on the adsorption mechanism. Low Temperature Physics, 2003, 29, 880-882.	0.6	20
40	Title is missing!. Journal of Low Temperature Physics, 2001, 122, 171-177.	1.4	8
41	On the Character of Atomic Adlayers Physiadsorbed on an Incommensurate Substrate. Journal of Low Temperature Physics, 2001, 122, 121-128.	1.4	9
42	Calculations on the stability of low temperature solid nitrogen phases. Journal of Chemical Physics, 2000, 112, 6745-6748.	3.0	5