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	Nanospace engineering of KOH activated carbon. Nanotechnology, 2012, 23, 015401.	2.6	301
2	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
3	Numerical estimation of hydrogen storage limits in carbon-based nanospaces. Carbon, 2010, 48, 223-231.	10.3	59
4	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
5	Enhanced hydrogen adsorption in boron substituted carbon nanospaces. Journal of Chemical Physics, 2009, 131, 164702.	3.0	50
6	Boron substituted graphene: energy landscape for hydrogen adsorption. Adsorption, 2009, 15, 312-317.	3.0	41
7	A review of boron enhanced nanoporous carbons for hydrogen adsorption: numerical perspective. Adsorption, 2010, 16, 413-421.	3.0	34
8	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
9	Understanding Universal Adsorption Limits for Hydrogen Storage in Nano Porous Systems. Advanced Materials, 2013, 25, 5971-5974.	21.0	28
10	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
11	Benchmarking of GGA density functionals for modeling structures of nanoporous, rigid and flexible MOFs. Journal of Chemical Physics, 2018, 149, 064110.	3.0	23
12	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
13	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
14	Increased H2 gravimetric storage capacity in truncated carbon slit pores modeled by Grand Canonical Monte Carlo. Carbon, 2013, 53, 208-215.	10.3	18
15	Modeling of low temperature adsorption of hydrogen in carbon nanopores. Journal of Molecular Modeling, 2017, 23, 20.	1.8	17
16	Engineered Porous Carbon for High Volumetric Methane Storage. Adsorption Science and Technology, 2014, 32, 681-691.	3.2	16
17	Open carbon frameworks - a search for optimal geometry for hydrogen storage. Journal of Molecular Modeling, 2013, 19, 4079-4087.	1.8	15
18	Influence of structural heterogeneity of nanoporous sorbent walls on hydrogen storage. Applied Surface Science, 2010, 256, 5270-5274.	6.1	14

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19	Melting of Hexane Monolayers Adsorbed on Graphite: The Role of Domains and Defect Formation. Langmuir, 2009, 25, 6596-6598.	3.5	13
20	Intermediate states approach for adsorption studies in flexible metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2019, 21, 3294-3303.	2.8	13
21	Effect of low frequency phonons on structural properties of ZIFs with SOD topology. Microporous and Mesoporous Materials, 2020, 304, 109132.	4.4	13
22	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
23	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
24	On the Character of Atomic Adlayers Physiadsorbed on an Incommensurate Substrate. Journal of Low Temperature Physics, 2001, 122, 121-128.	1.4	9
25	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
26	Title is missing!. Journal of Low Temperature Physics, 2001, 122, 171-177.	1.4	8
27	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
28	Simulation and Characterization of Tetracosane on Graphite: Molecular Dynamics Beyond the Monolayer. Journal of Physical Chemistry C, 2016, 120, 984-994.	3.1	7
29	Phonons in deformable microporous crystalline solids. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 513-527.	0.8	7
30	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
31	Calculations on the stability of low temperature solid nitrogen phases. Journal of Chemical Physics, 2000, 112, 6745-6748.	3.0	5
32	Absorption of atomic and molecular species in carbon cellular structures (Review article). Low Temperature Physics, 2020, 46, 219-231.	0.6	5
33	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
34	Molecular dynamics simulations of submonolayer hexane and pentane films on graphite. Molecular Simulation, 2010, 36, 326-333.	2.0	3
35	Hydrogen adsorption on surfaces with different binding energies. Chemical Data Collections, 2016, 2, 56-60.	2.3	3
36	How dense is the gas adsorbed in nanopores?. Microporous and Mesoporous Materials, 2020, 304, 109240.	4.4	3

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37	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
38	Hydrogen Storage in Pure and Boron-Substituted Nanoporous Carbonsâ€"Numerical and Experimental Perspective. Nanomaterials, 2021, 11, 2173.	4.1	3
39	Influence of Strength of Atom-Wall Interactions on Adsorption Mechanism. Adsorption, 2005, 11, 367-372.	3.0	2
40	Evolution of methane density during melting in nanopores. Journal of Molecular Modeling, 2017, 23, 44.	1.8	2
41	Computer modeling of 2D supramolecular nanoporous monolayers self-assembled on graphite. Nanoscale, 2019, 11, 21284-21290.	5.6	2
42	Hydrogen Storage in Pure and Boron-Substituted Nanoporous Carbons-Numerical and Experimental Perspective. Nanomaterials, 2021, 11, .	4.1	0