Lev Sarkisov

List of Publications by Year
in descending order

71	4,205	147786 31	110368 64
papers	citations	h-index	g-index

73	73	73	4403
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Performance-based ranking of porous materials for PSA carbon capture under the uncertainty of experimental data. Chemical Engineering Journal, 2022, 437, 135395.	12.7	9
2	Lattice Model of Fluid Transport in Mixed Matrix Membranes. Advanced Theory and Simulations, 2022, 5, .	2.8	3
3	MOF materials as therapeutic agents, drug carriers, imaging agents and biosensors in cancer biomedicine: Recent advances and perspectives. Progress in Materials Science, 2021, 117, 100743.	32.8	120
4	Water Dynamics in NH₂-MIL-125: Insights from a Combined ¹H NMR Relaxometry and Computational Investigation. Journal of Physical Chemistry C, 2021, 125, 14416-14429.	3.1	1
5	Activity coefficient models for accurate prediction of adsorption azeotropes. Adsorption, 2021, 27, 1191-1206.	3.0	6
6	Application of the dynamic mean field theory to fluid transport in slit pores. Journal of Chemical Physics, 2021, 155, 074702.	3.0	4
7	Performance-Based Screening of Porous Materials for Carbon Capture. Chemical Reviews, 2021, 121, 10666-10741.	47.7	115
8	Nanostructures of Ionic Liquids Confined in Pores of SBA-15: Insights from Experimental Studies and Mean-Field Density Functional Theory. Journal of Physical Chemistry C, 2021, 125, 21254-21269.	3.1	5
9	Competitive H2S â€“ CO2 absorption in reactive aqueous methyldiethanolamine solution: Prediction with ePC-SAFT. Fluid Phase Equilibria, 2020, 511, 112453.	2.5	18
10	Materials Informatics with PoreBlazer v4.0 and the CSD MOF Database. Chemistry of Materials, 2020, 32, 9849-9867.	6.7	132
11	On competitive gas adsorption and absorption phenomena in thin films of ionic liquids. Journal of Materials Chemistry A, 2020, 8, 11781-11799.	10.3	25
12	Exploring new sources of efficiency in process-driven materials screening for post-combustion carbon capture. Energy and Environmental Science, 2020, 13, 1018-1037.	30.8	35
13	On the Universality of Capillary Condensation and Adsorption Hysteresis Phenomena in Ordered and Crystalline Mesoporous Materials. Advanced Materials Interfaces, 2020, 7, 2000184.	3.7	23
14	Guest-dependent negative thermal expansion in a lanthanide-based metalâ€“organic framework. CrystEngComm, 2019, 21, 5292-5298.	2.6	4
15	Exploring the thermodynamic criteria for responsive adsorption processes. Chemical Science, 2019, 10, 5011-5017.	7.4	29
16	Deciphering the Relations between Pore Structure and Adsorption Behavior in Metalâ€“Organic Frameworks: Unexpected Lessons from Argon Adsorption on Copperâ€“Benzene-1,3,5-tricarboxylate. Journal of the American Chemical Society, 2019, 141, 8397-8401.	13.7	30
17	Structure and dynamics of water in molecular models of hydrated polyvinylamine membranes. Physical Chemistry Chemical Physics, 2019, 21, 26453-26465.	2.8	6
18	Solubility prediction in mixed solvents: A combined molecular simulation and experimental approach. Fluid Phase Equilibria, 2019, 484, 26-37.	2.5	4

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19	Nanomaterial interactions with biomembranes: Bridging the gap between soft matter models and biological context. Biointerphases, 2018, 13, 028501.	1.6	23
20	Automated analysis and benchmarking of GCMC simulation programs in application to gas adsorption. Molecular Simulation, 2018, 44, 309-321.	2.0	21
21	From Crystal to Adsorption Column: Challenges in Multiscale Computational Screening of Materials for Adsorption Separation Processes. Industrial & Engineering Chemistry Research, 2018, 57, 15491-15511.	3.7	61
22	Thermodynamics 2017 Conference â€" Edinburgh, Scotland, 5â€"8 September 2017. Molecular Physics, 2018, 116, 1909-1914.	1.7	2
23	Improving the Mechanical Stability of Metalâ€"Organic Frameworks Using Chemical Caryatids. ACS Central Science, 2018, 4, 832-839.	11.3	67
24	Molecular simulation and experiments of water adsorption in a high surface area activated carbon: Hysteresis, scanning curves and spatial organization of water clusters. Carbon, 2017, 118, 127-138.	10.3	49
25	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	3.2	4
26	Ethanolamine Purification by Nanofiltration through PIM-1 and Carbon Membranes: A Molecular Simulation Study. Journal of Physical Chemistry C, 2017, 121, 20539-20545.	3.1	11
27	Self-assembly of anionic, ligand-coated nanoparticles in lipid membranes. Nanoscale, 2017, 9, 1040-1048.	5.6	50
28	Net, excess and absolute adsorption and adsorption of helium. Adsorption, 2016, 22, 261-276.	3.0	75
29	Molecular simulation of perfluorohexane adsorption in BAM-P109 activated carbon. Adsorption Science and Technology, 2016, 34, 42-63.	3.2	4
30	Molecular simulation of low temperature argon adsorption in several models of IRMOF-1 with defects and structural disorder. Dalton Transactions, 2016, 45, 4203-4212.	3.3	25
31	Computational structure characterization tools for the era of material informatics. Chemical Engineering Science, 2015, 121, 322-330.	3.8	29
32	Molecular simulation of multi-component adsorption processes related to carbon capture in a high surface area, disordered activated carbon. Carbon, 2015, 94, 27-40.	10.3	38
33	Membrane Partitioning of Anionic, Ligand-Coated Nanoparticles Is Accompanied by Ligand Snorkeling, Local Disordering, and Cholesterol Depletion. PLoS Computational Biology, 2014, 10, e1003917.	3.2	59
34	Computer Simulation Studies of Adsorption of Binary and Ternary Mixtures of Gasoline Components in Engine Deposits. SAE International Journal of Fuels and Lubricants, 2014, 7, 756-761.	0.2	4
35	Branched versus linear alkane adsorption in carbonaceous slit pores. Adsorption, 2014, 20, 427-437.	3.0	31
36	On the Flexibility of Metalâ€"Organic Frameworks. Journal of the American Chemical Society, 2014, 136, 2228-2231.	13.7	198

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37	Effective interactions in molecular dynamics simulations of lysozyme solutions. European Physical Journal B, 2014, 87, 1.	1.5	3
38	Systematic development of predictive molecular models of high surface area activated carbons for adsorption applications. Carbon, 2013, 64, 262-280.	10.3	76
39	Experiences with the publicly available multipurpose simulation code, Music. Molecular Simulation, 2013, 39, 1223-1232.	2.0	33
40	Homogeneous Hydrophobicâ€“Hydrophilic Surface Patterns Enhance Permeation of Nanoparticles through Lipid Membranes. Journal of Physical Chemistry Letters, 2013, 4, 1907-1912.	4.6	67
41	Calculation and visualization of free energy barriers for several VOCs and TNT in HKUST-1. Physical Chemistry Chemical Physics, 2012, 14, 15438.	2.8	13
42	Toward Rational Design of Metalâ€“Organic Frameworks for Sensing Applications: Efficient Calculation of Adsorption Characteristics in Zero Loading Regime. Journal of Physical Chemistry C, 2012, 116, 3025-3033.	3.1	48
43	Accessible Surface Area of Porous Materials: Understanding Theoretical Limits. Advanced Materials, 2012, 24, 3130-3133.	21.0	54
44	Structure and Phase Transformations of DPPC Lipid Bilayers in the Presence of Nanoparticles: Insights from Coarse-Grained Molecular Dynamics Simulations. Langmuir, 2011, 27, 3723-3730.	3.5	80
45	Editorial [Hot Topic: Multiscale Modelling of Biomembrane Interactions with Nano-Objects (Guest) Tj ETQq1 1 0.784314 rgBT /Overlo	1.2	1
46	Towards predictive molecular simulations of normal and branched alkane adsorption in carbonaceous engine deposits. Carbon, 2011, 49, 445-456.	10.3	14
47	Computational structure characterisation tools in application to ordered and disordered porous materials. Molecular Simulation, 2011, 37, 1248-1257.	2.0	548
48	Molecular Recognition Effects in Atomistic Models of Imprinted Polymers. International Journal of Molecular Sciences, 2011, 12, 4781-4804.	4.1	13
49	The Role of Hydrophobicity in Peptide-Membrane Interactions: Insights Through Coarse-Grained Molecular Dynamics Simulations. Biophysical Journal, 2010, 98, 82a.	0.5	0
50	Interactions of Phospholipid Bilayers with Several Classes of Amphiphilic Î±-Helical Peptides: Insights from Coarse-Grained Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 826-839.	2.6	55
51	Emergence of molecular recognition phenomena in a simple model of imprinted porous materials. Journal of Chemical Physics, 2009, 130, 214701.	3.0	14
52	Structural characterization of carbonaceous combustion-chamber deposits. Carbon, 2009, 47, 3322-3331.	10.3	10
53	Computer Simulation of Volatile Organic Compound Adsorption in Atomistic Models of Molecularly Imprinted Polymers. Langmuir, 2009, 25, 5352-5359.	3.5	65
54	Spontaneous Formation of a Barrel-Stave Pore in a Coarse-Grained Model of the Synthetic LS3 Peptide and a DPPC Lipid Bilayer. Journal of Physical Chemistry B, 2009, 113, 6-8.	2.6	25

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55	Computer simulation of adsorption in simple models of molecularly imprinted polymers. , 2009, , .		1
56	Theories of molecular fluids confined in disordered porous materials. Journal of Physics Condensed Matter, 2008, 20, 333101.	1.8	13
57	Theory of pair connectedness in templated quenched-annealed systems. Journal of Chemical Physics, 2008, 128, 044707.	3.0	7
58	Molecular Dynamics Characterization of Protein Crystal Contacts in Aqueous Solutions. Physical Review Letters, 2008, 101, 248102.	7.8	38
59	Solution-Phase Structural Characterization of Supramolecular Assemblies by Molecular Diffraction. Journal of the American Chemical Society, 2007, 129, 1578-1585.	13.7	47
60	Integral Equation Theory of Adsorption in Templated Materials:â€‰ Influence of Molecular Attraction. Journal of Physical Chemistry C, 2007, 111, 15726-15735.	3.1	14
61	Molecular Squares, Rectangles, and Corners:Â Ground-State Electronic Structure and Configurational Properties. Chemistry of Materials, 2006, 18, 620-628.	6.7	1
62	Replica Ornstein-Zernike theory of adsorption in a templated porous material: Interaction site systems. Journal of Chemical Physics, 2005, 123, 164706.	3.0	27
63	Molecular modelling of adsorption in novel nanoporous metalâ€“organic materials. Molecular Physics, 2004, 102, 211-221.	1.7	126
64	Structural analysis of porphyrin molecular squares using molecular mechanics and density-functional methods. Journal of Chemical Physics, 2004, 121, 7228-7236.	3.0	13
65	Design of New Materials for Methane Storage. Langmuir, 2004, 20, 2683-2689.	3.5	663
66	Modeling of Adsorption and Desorption in Pores of Simple Geometry Using Molecular Dynamics. Langmuir, 2001, 17, 7600-7604.	3.5	247
67	Mean-Field Theory of Fluid Adsorption in a Porous Glass. Langmuir, 2001, 17, 7472-7475.	3.5	83
68	Capillary Condensation in Disordered Porous Materials: Hysteresis versus Equilibrium Behavior. Physical Review Letters, 2001, 87, 055701.	7.8	261
69	Lattice model of adsorption in disordered porous materials: Mean-field density functional theory and Monte Carlo simulations. Physical Review E, 2001, 65, 011202.	2.1	80
70	Computer simulations of phase equilibrium for a fluid confined in a disordered porous structure. Physical Review E, 2000, 61, 7231-7234.	2.1	59
71	Hysteresis in Monte Carlo and Molecular Dynamics Simulations of Adsorption in Porous Materials. Langmuir, 2000, 16, 9857-9860.	3.5	83