Libo Li

List of Publications by Year in Descending Order

72 papers	3,537 citations	27 h-index	59 g-index
73 ext. papers	4,426 ext. citations	5.5 avg, IF	5.87 L-index

#	Paper	IF	Citations
72	Recent advances in the synthesis of nanoscale hierarchically porous metal–organic frameworks. *Nano Materials Science*, **2022**,	10.2	2
71	Application of hierarchically porous metal-organic frameworks in heterogeneous catalysis: A review. *Science China Materials*, **2022**, 65, 298-320	7.1	7
70	Lysozyme Adsorption on Different Functionalized MXenes: A Multiscale Simulation Study. *Langmuir* , **2021**, 37, 5932-5942	4	0
69	Molecular dynamics simulation on DNA translocating through MoS2 nanopores with various structures. *Frontiers of Chemical Science and Engineering*, **2021**, 15, 922-934	4.5	2
68	Recent advances in the synthesis of monolithic metal-organic frameworks. *Science China Materials*, **2021**, 64, 1305-1319	7.1	51
67	Identical Composition and Distinct Performance: How ZIF-8 Polymorphs' Structures Affect the Adsorption/Separation of Ethane and Ethene. *Journal of Chemical & Engineering Data*, **2021**, 66, 3483-3492	2.8	3
66	Effective ion sieving with Ti3C2Tx MXene membranes for production of drinking water from seawater. *Nature Sustainability*, **2020**, 3, 296-302	22.1	204
65	Atomic Force Microscopy and Molecular Dynamics Simulations for Study of Lignin Solution Self-Assembly Mechanisms in Organic-Aqueous Solvent Mixtures. *ChemSusChem*, **2020**, 13, 4420-4427	8.3	43
64	Water-based routes for synthesis of metal-organic frameworks: A review. *Science China Materials*, **2020**, 63, 667-685	7.1	103
63	Solvent effect on xylose conversion under catalyst-free conditions: insights from molecular dynamics simulation and experiments. *Green Chemistry*, **2020**, 22, 532-539	10	22
62	Engineering New Defects in MIL-100(Fe) via a Mixed-Ligand Approach To Effect Enhanced Volatile Organic Compound Adsorption Capacity. *Industrial & Engineering Chemistry Research*, **2020**, 59, 774-782	3.9	69
61	Adsorption and separation of propane/propylene on various ZIF-8 polymorphs: Insights from GCMC simulations and the ideal adsorbed solution theory (IAST). *Chemical Engineering Journal*, **2020**, 386, 123945	14.7	21
60	Lysozyme Adsorption on Porous Organic Cages: A Molecular Simulation Study. *Langmuir*, **2020**, 36, 12299-12308	4	9
59	Surface Regulation Towards Stimuli-Responsive Luminescence of Ultrasmall Thiolated Gold Nanoparticles for Ratiometric Imaging. *Advanced Functional Materials*, **2019**, 29, 1806945	15.6	26
58	Ultra-thin titanium carbide (MXene) sheet membranes for high-efficient oil/water emulsions separation. *Journal of Membrane Science*, **2019**, 592, 117361	9.6	54
57	Salt effect on the liquid–liquid equilibrium of the ternary (water + phenol + methyl isobutyl ketone) system: Experimental data and correlation. *Chinese Journal of Chemical Engineering*, **2019**, 27, 168-173	3.2	4
56	Hierarchically structured metal–organic frameworks assembled by hydroxy double salt–template synergy with high space–time yields. *CrystEngComm*, **2018**, 20, 1057-1064	3.3	32

55	MXene molecular sieving membranes for highly efficient gas separation. *Nature Communications*, **2018**, 9, 155	17.4	530
54	Computer Simulation of DNA Condensation by PAMAM Dendrimer. *Macromolecular Theory and Simulations*, **2018**, 27, 1700070	1.5	13
53	Protein Translocation through a MoS2 Nanopore:A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2018**, 122, 2070-2080	3.8	32
52	Simulation insight into the cytochrome c adsorption on graphene and graphene oxide surfaces. *Applied Surface Science*, **2018**, 428, 825-834	6.7	25
51	Measurement and correlation of phase equilibrium data of the mixtures consisting of water, resorcinol, mesityl oxide at different temperatures. *Chinese Journal of Chemical Engineering*, **2018**, 26, 2573-2580	3.2	8
50	Liquid-liquid equilibrium for methyl butyl ketone + o-, m-, p-cresol + water ternary systems and COSMO-SAC predictions. *Journal of Chemical Thermodynamics*, **2018**, 127, 17-24	2.9	13
49	Facile synthesis of hierarchical porous metal-organic frameworks with enhanced catalytic activity. *Chemical Engineering Journal*, **2018**, 334, 1477-1483	14.7	67
48	Ethane/ethylene separation in a metal-organic framework with iron-peroxo sites. *Science*, **2018**, 362, 443-446	33.3	478
47	Paralyzed membrane: Current-driven synthesis of a metal-organic framework with sharpened propene/propane separation. *Science Advances*, **2018**, 4, eaau1393	14.3	132
46	Selective gas diffusion in two-dimensional MXene lamellar membranes: insights from molecular dynamics simulations. *Journal of Materials Chemistry A*, **2018**, 6, 11734-11742	13	61
45	Computer simulations on the pH-sensitive tri-block copolymer containing zwitterionic sulfobetaine as a novel anti-cancer drug carrier. *Colloids and Surfaces B: Biointerfaces*, **2017**, 152, 260-268	6	37
44	Liquid□liquid Equilibrium for the Ternary Systems Methyl tert-Butyl Ketone + o-, m-, p-Cresol + Water at (298.2, 313.2, and 323.2) K. *Journal of Chemical & Engineering Data*, **2017**, 62, 1929-1936	2.8	5
43	Water Transport with Ultralow Friction through Partially Exfoliated g-C N Nanosheet Membranes with Self-Supporting Spacers. *Angewandte Chemie - International Edition*, **2017**, 56, 8974-8980	16.4	177
42	Liquid phase equilibrium of the ternary systems, water + propionic or butyric acid + mesityl oxide, at (298.2 and 323.2) K. *Journal of Chemical Thermodynamics*, **2017**, 111, 72-79	2.9	15
41	Measurement, correlation and COSMO-SAC prediction of liquid-liquid equilibrium for the ternary systems, mesityl oxide□+□o-, m-, p-cresol□+□water, at 333.2K and 353.2□K. *Fluid Phase Equilibria*, **2017**, 440, 45-53	2.5	14
40	Phase Equilibrium Measurement and Thermodynamic Modeling of the 4-Methylpentan-2-one/3-Methylphenol, and 4-Methylphenol/Water Ternary Systems at 298.2, 313.2, and 323.2 K and 0.1 MPa. *Journal of Chemical & Engineering Data*, **2017**, 62, 141-147	2.8	4
39	Liquid-liquid equilibrium for ternary systems, methyl isobutyl ketone + (catechol, resorcinol and hydroquinone) + water at 333.15 K, 343.15 K and 353.15 K. *Fluid Phase Equilibria*, **2017**, 433, 206-211	2.5	11
38	Computer Simulations on the Channel Membrane Formation by Nonsolvent Induced Phase Separation. *Macromolecular Theory and Simulations*, **2017**, 26, 1700027	1.5	14

37	Extraction of o-, m- and p-cresol from aqueous solution with methyl isopropyl ketone: Equilibrium, correlations, and COSMO-RS predictions. *Journal of Chemical Thermodynamics*, **2017**, 115, 180-190	2.9	14
36	Screening solvents to extract phenol from aqueous solutions by the COSMO-SAC model and extraction process simulation. *Fluid Phase Equilibria*, **2017**, 451, 12-24	2.5	29
35	Understanding the Cellular Uptake of pH-Responsive Zwitterionic Gold Nanoparticles: A Computer Simulation Study. *Langmuir*, **2017**, 33, 14480-14489	4	20
34	Liquid–liquid Equilibrium of Ternary Systems of Methyl Isobutyl Ketone + o-Cresol + Water at 298.2, 313.2 and 323.2 K. *Journal of Solution Chemistry*, **2017**, 46, 2204-2213	1.8	4
33	Molecular Understanding of the Penetration of Functionalized Gold Nanoparticles into Asymmetric Membranes. *Langmuir*, **2017**, 33, 361-371	4	38
32	Measurement and thermodynamic modeling of ternary (liquid + liquid) equilibrium for extraction of o-cresol, m-cresol or p-cresol from aqueous solution with 2-pentanone. *Journal of Chemical Thermodynamics*, **2017**, 104, 230-238	2.9	22
31	Phase Behavior of an Amphiphilic Block Copolymer in Ionic Liquid: A Dissipative Particle Dynamics Study. *Journal of Chemical & Engineering Data*, **2016**, 61, 3998-4005	2.8	17
30	Experimental Determination and Correlation of Liquid–liquid Equilibria for Methyl Isopropyl Ketone + Phenol + Water Mixtures at 298.15, 313.15, and 323.15 K. *Journal of Chemical & Engineering Data*, **2016**, 61, 2221-2225	2.8	18
29	Measurement and Correlation of Liquid–liquid Equilibria for the Ternary Methyl Isobutyl Ketone + Phenol + Water System at (333.15, 343.15 and 353.15) K under Atmospheric Pressure. *Journal of Solution Chemistry*, **2016**, 45, 875-884	1.8	14
28	Ternary and Quaternary Liquid–liquid Equilibria for Systems of Methyl Butyl Ketone + Water + Hydroquinone + Phenol at 313.2 K and Atmospheric Pressure. *Journal of Chemical & Engineering Data*, **2016**, 61, 1540-1546	2.8	7
27	Tie-Line Data for Aqueous Mixtures of Butyric Acid with Diisopropyl Ether at Various Temperatures. *Journal of Chemical & Engineering Data*, **2016**, 61, 760-765	2.8	6
26	Measurements and thermodynamic modeling of liquid–liquid equilibria in ternary system 2-methoxy-2-methylpropane+p-cresol+water. *Chinese Journal of Chemical Engineering*, **2016**, 24, 360-364	3.2	13
25	Liquid–liquid Equilibria for the Ternary System Mesityl Oxide + Phenol + Water at 298.15, 313.15, and 323.15 K. *Journal of Chemical & Engineering Data*, **2016**, 61, 2493-2498	2.8	27
24	Molecular dynamics simulations of conformation changes of HIV-1 regulatory protein on graphene. *Applied Surface Science*, **2016**, 377, 324-334	6.7	34
23	Phase Equilibrium for Phenol Extraction from Aqueous Solution with 2-Pentanone at Different Temperatures. *Journal of Solution Chemistry*, **2016**, 45, 1414-1424	1.8	14
22	Ternary liquid–liquid equilibria for methyl isopropyl ketone + (resorcinol or hydroquinone) + water systems at different temperatures. *Fluid Phase Equilibria*, **2016**, 429, 93-97	2.5	22
21	Determination and modeling of liquid-liquid equilibrium for ternary mixtures of methyl isopropyl ketone, cresol isomers and water. *Fluid Phase Equilibria*, **2016**, 429, 107-112	2.5	21
20	Liquid-liquid equilibria for methyl isobutyl ketone + cresols + water at 333.15 K, 343.15 K and 353.15 K: Experimental results and data correlation. *Fluid Phase Equilibria*, **2016**, 427, 291-296	2.5	25

19	Liquid–liquid equilibria in the ternary systems water + cresols + methyl butyl ketone at 298.2 and 313.2 K: Experimental data and correlation. *Fluid Phase Equilibria*, **2015**, 404, 89-95	2.5	27
18	Experimental Determination and Correlation of Liquid–liquid Equilibria for the Ternary System 2-Methoxy-2-methylpropane + o-Cresol + Water at 298.15 K and 313.15 K. *Journal of Chemical & Engineering Data*, **2015**, 60, 1396-1400	2.8	24
17	Liquid–liquid Phase Equilibria for the Ternary Water + Acetic Acid + 3,3-Dimethyl-2-butanone System at (298.15, 313.15 and 323.15) K. *Journal of Chemical & Engineering Data*, **2015**, 60, 3187-3192	2.8	1
16	Ternary Liquid–liquid Equilibria for the System 2-Methoxy-2-methylpropane + m-Cresol + Water at 298.15 and 313.15 K: Experimental Data and Correlation. *Journal of Solution Chemistry*, **2015**, 44, 2393-2404	1.8	13
15	Phase equilibria of (water + propionic acid or butyric acid + 2-methoxy-2-methylpropane) ternary systems at 298.2 K and 323.2 K. *Fluid Phase Equilibria*, **2015**, 403, 30-35	2.5	26
14	Field-SEA: a model for computing the solvation free energies of nonpolar, polar, and charged solutes in water. *Journal of Physical Chemistry B*, **2014**, 118, 6431-7	3.4	27
13	Liquid–liquid Equilibria for Ternary Systems: Methyl Butyl Ketone + Phenol + Water and Methyl Butyl Ketone + Hydroquinone + Water at 298.15 K and 323.15 K. *Journal of Chemical & Engineering Data*, **2014**, 59, 2750-2755	2.8	44
12	Testing the semi-explicit assembly model of aqueous solvation in the SAMPL4 challenge. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 259-64	4.2	8
11	Small molecule solvation changes due to the presence of salt are governed by the cost of solvent cavity formation and dispersion. *Journal of Chemical Physics*, **2014**, 141, 22D518	3.9	7
10	The different interactions of lysine and arginine side chains with lipid membranes. *Journal of Physical Chemistry B*, **2013**, 117, 11906-20	3.4	176
9	The role of membrane thickness in charged protein-lipid interactions. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 135-45	3.8	55
8	Simple liquid models with corrected dielectric constants. *Journal of Physical Chemistry B*, **2012**, 116, 6936-44	3.4	54
7	Assessing atomistic and coarse-grained force fields for protein-lipid interactions: the formidable challenge of an ionizable side chain in a membrane. *Journal of Physical Chemistry B*, **2008**, 112, 9588-602	3.4	99
6	Potential of mean force and pKa profile calculation for a lipid membrane-exposed arginine side chain. *Journal of Physical Chemistry B*, **2008**, 112, 9574-87	3.4	102
5	Is arginine charged in a membrane?. *Biophysical Journal*, **2008**, 94, L11-3	2.9	74
4	Chapter 15 Charged Protein Side Chain Movement in Lipid Bilayers Explored with Free Energy Simulation. *Current Topics in Membranes*, **2008**, 405-459	2.2	2
3	A simple model for growth of semiconductor nanorods using lamellar precursors. *Materials Chemistry and Physics*, **2005**, 94, 1-6	4.4	9
2	Novel inorganic-organic-layered structures: crystallographic understanding of both phase and morphology formations of one-dimensional CdE (E = S, Se, Te) nanorods in ethylenediamine. *Inorganic Chemistry*, **2003**, 42, 2331-41	5.1	156

1	Solvent effect on xylose-to-furfural reaction in biphasic systems: combined experiments with theoretical calculations. *Green Chemistry*,	10	6