Reid C Van Lehn

List of Publications by Year
in descending order

50	1,741	331670 21	289244 40
papers	citations	h-index	g-index

54	54	54	2071
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Identifying nonadditive contributions to the hydrophobicity of chemically heterogeneous surfaces via dual-loop active learning. Journal of Chemical Physics, 2022, 156, 024701.	3.0	6
2	On the integration of molecular dynamics, data science, and experiments for studying solvent effects on catalysis. Current Opinion in Chemical Engineering, 2022, 36, 100796.	7.8	4
3	Predicting the Physicochemical Properties and Biological Activities of Monolayer-Protected Gold Nanoparticles Using Simulation-Derived Descriptors. ACS Nano, 2022, 16, 6282-6292.	14.6	13
4	Adaptive Conformer Sampling for Property Prediction Using the Conductor-like Screening Model for Real Solvents. Industrial & Engineering Chemistry Research, 2022, 61, 9025-9036.	3.7	5
5	The Interplay of Ligand Properties and Core Size Dictates the Hydrophobicity of Monolayer-Protected Gold Nanoparticles. ACS Nano, 2021, 15, 4534-4545.	14.6	22
6	Molecular simulations of lipid membrane partitioning and translocation by bacterial quorum sensing modulators. PLoS ONE, 2021, 16, e0246187.	2.5	13
7	Membrane Remodeling and Stimulation of Aggregation Following Î±-Synuclein Adsorption to Phosphotidylserine Vesicles. Journal of Physical Chemistry B, 2021, 125, 1582-1594.	2.6	16
8	Lipophilicity of Cationic Ligands Promotes Irreversible Adsorption of Nanoparticles to Lipid Bilayers. ACS Nano, 2021, 15, 6562-6572.	14.6	27
9	Analysis of Charged Peptide Loop-Flipping across a Lipid Bilayer Using the String Method with Swarms of Trajectories. Journal of Physical Chemistry B, 2021, 125, 5862-5873.	2.6	3
10	Bacterial Quorum Sensing Signals Promote Large-Scale Remodeling of Lipid Membranes. Langmuir, 2021, 37, 9120-9136.	3.5	10
11	Computational Approach for Rapidly Predicting Temperatureâ€Dependent Polymer Solubilities Using Molecularâ€Scale Models. ChemSusChem, 2021, 14, 4307-4316.	6.8	15
12	Predicting Critical Micelle Concentrations for Surfactants Using Graph Convolutional Neural Networks. Journal of Physical Chemistry B, 2021, 125, 10610-10620.	2.6	12
13	Reducing Antisolvent Use in the STRAP Process by Enabling a Temperatureâ€Controlled Polymer Dissolution and Precipitation for the Recycling of Multilayer Plastic Films. ChemSusChem, 2021, 14, 4317-4329.	6.8	29
14	Interactions of Bacterial Quorum Sensing Signals with Model Lipid Membranes: Influence of Acyl Tail Structure on Multiscale Response. Langmuir, 2021, 37, 12049-12058.	3.5	3
15	Molecular simulations of analyte partitioning and diffusion in liquid crystal sensors. Molecular Systems Design and Engineering, 2020, 5, 304-316.	3.4	14
16	Effect of Mixed-Solvent Environments on the Selectivity of Acid-Catalyzed Dehydration Reactions. ACS Catalysis, 2020, 10, 1679-1691.	11.2	45
17	Recycling of multilayer plastic packaging materials by solvent-targeted recovery and precipitation. Science Advances, 2020, 6, .	10.3	170
18	Fast predictions of liquid-phase acid-catalyzed reaction rates using molecular dynamics simulations and convolutional neural networks. Chemical Science, 2020, 11, 12464-12476.	7.4	24

#	Article	IF	Citations
19	Predicting Hydrophobicity by Learning Spatiotemporal Features of Interfacial Water Structure: Combining Molecular Dynamics Simulations with Convolutional Neural Networks. Journal of Physical Chemistry B, 2020, 124, 9103-9114.	2.6	21
20	Bilayerâ€mediated assembly of cationic nanoparticles adsorbed to lipid bilayers: Insights from molecular simulations. AICHE Journal, 2020, 66, e16993.	3.6	1
21	Solvent Selection for the Separation of Lignin-Derived Monomers Using the Conductor-like Screening Model for Real Solvents. Industrial & Engineering Chemistry Research, 2020, 59, 7755-7764.	3.7	17
22	Rational Design of Mixed Solvent Systems for Acid-Catalyzed Biomass Conversion Processes Using a Combined Experimental, Molecular Dynamics and Machine Learning Approach. Topics in Catalysis, 2020, 63, 649-663.	2.8	11
23	Bacterial Quorum Sensing Signals Self-Assemble in Aqueous Media to Form Micelles and Vesicles: An Integrated Experimental and Molecular Dynamics Study. Journal of Physical Chemistry B, 2020, 124, 3616-3628.	2.6	12
24	Quantifying the Stability of the Hydronium Ion in Organic Solvents With Molecular Dynamics Simulations. Frontiers in Chemistry, 2019, 7, 439.	3.6	13
25	Spatially Heterogeneous Water Properties at Disordered Surfaces Decrease the Hydrophobicity of Nonpolar Self-Assembled Monolayers. Journal of Physical Chemistry Letters, 2019, 10, 3991-3997.	4.6	20
26	Solvent-Mediated Affinity of Polymer-Wrapped Single-Walled Carbon Nanotubes for Chemically Modified Surfaces. Langmuir, 2019, 35, 12492-12500.	3.5	8
27	Curvature-driven adsorption of cationic nanoparticles to phase boundaries in multicomponent lipid bilayers. Nanoscale, 2019, 11, 2767-2778.	5.6	33
28	Energy landscape for the insertion of amphiphilic nanoparticles into lipid membranes: A computational study. PLoS ONE, 2019, 14, e0209492.	2.5	31
29	Molecular Order Affects Interfacial Water Structure and Temperature-Dependent Hydrophobic Interactions between Nonpolar Self-Assembled Monolayers. Langmuir, 2019, 35, 2078-2088.	3.5	38
30	Structureâ€“Property Relationships of Amphiphilic Nanoparticles That Penetrate or Fuse Lipid Membranes. Bioconjugate Chemistry, 2018, 29, 1131-1140.	3.6	36
31	Nanomaterial interactions with biomembranes: Bridging the gap between soft matter models and biological context. Biointerphases, 2018, 13, 028501.	1.6	23
32	Universal kinetic solvent effects in acid-catalyzed reactions of biomass-derived oxygenates. Energy and Environmental Science, 2018, 11, 617-628.	30.8	122
33	Random copolymers that protect proteins. Science, 2018, 359, 1216-1217.	12.6	4
34	Characterizing the Molecular Mechanisms for Flipping Charged Peptide Flanking Loops across a Lipid Bilayer. Journal of Physical Chemistry B, 2018, 122, 10337-10348.	2.6	5
35	Effect of Core Morphology on the Structural Asymmetry of Alkanethiol Monolayer-Protected Gold Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 26288-26297.	3.1	22
36	Grafting Charged Species to Membrane-Embedded Scaffolds Dramatically Increases the Rate of Bilayer Flipping. ACS Central Science, 2017, 3, 186-195.	11.3	16

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37	Influence of Order within Nonpolar Monolayers on Hydrophobic Interactions. Langmuir, 2017, 33, 4628-4637.	3.5	27
38	Structurally detailed coarse-grained model for Sec-facilitated co-translational protein translocation and membrane integration. PLoS Computational Biology, 2017, 13, e1005427.	3.2	22
39	Solvent-exposed lipid tail protrusions depend on lipid membrane composition and curvature. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1207-1215.	2.6	23
40	Pathway for insertion of amphiphilic nanoparticles into defect-free lipid bilayers from atomistic molecular dynamics simulations. Soft Matter, 2015, 11, 3165-3175.	2.7	57
41	Regulation of multispanning membrane protein topology via post-translational annealing. ELife, 2015, 4, .	6.0	42
42	Membrane-Embedded Nanoparticles Induce Lipid Rearrangements Similar to Those Exhibited by Biological Membrane Proteins. Journal of Physical Chemistry B, 2014, 118, 12586-12598.	2.6	48
43	Free energy change for insertion of charged, monolayer-protected nanoparticles into lipid bilayers. Soft Matter, 2014, 10, 648-658.	2.7	58
44	Lipid tail protrusions mediate the insertion of nanoparticles into model cell membranes. Nature Communications, 2014, 5, 4482.	12.8	183
45	Fusion of Ligand-Coated Nanoparticles with Lipid Bilayers: Effect of Ligand Flexibility. Journal of Physical Chemistry A, 2014, 118, 5848-5856.	2.5	43
46	Ligand-Mediated Short-Range Attraction Drives Aggregation of Charged Monolayer-Protected Gold Nanoparticles. Langmuir, 2013, 29, 8788-8798.	3.5	48
47	Effect of Particle Diameter and Surface Composition on the Spontaneous Fusion of Monolayer-Protected Gold Nanoparticles with Lipid Bilayers. Nano Letters, 2013, 13, 4060-4067.	9.1	236
48	Structure of Mixed-Monolayer-Protected Nanoparticles in Aqueous Salt Solution from Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2013, 117, 20104-20115.	3.1	63
49	Communication: Lateral phase separation of mixed polymer brushes physisorbed on planar substrates. Journal of Chemical Physics, 2011, 135, 141106.	3.0	20
50	A simple simulation-derived descriptor for the deposition of polymer-wrapped carbon nanotubes on functionalized substrates. Soft Matter, 0, , .	2.7	0