Jeffery B Klauda

List of Publications by Year
in descending order

148 papers	16,033 citations	57681 46 h-index	21843 118 g-index
155 all docs	155 docs citations	155 times ranked	15369 citing authors

#	Article	IF	Citations
1	Experimental investigation of the mechanism of lipid-binding of the ALPS-like motif of Osh4 protein. Biophysical Journal, 2022, 121, 221a-222a.	0.2	0
2	Modeling the membrane binding mechanism of a lipid transport protein Osh4 to single membranes. Biophysical Journal, 2022, 121, 1560-1575.	0.2	4
3	All-Atom Modeling of Complex Cellular Membranes. Langmuir, 2022, 38, 3-17.	1.6	6
4	Leaflet Asymmetry Modeling in the Lipid Composition of Escherichia coli Cytoplasmic Membranes. Journal of Physical Chemistry B, 2022, 126, 184-196.	1.2	4
5	GraphVAMPNet, using graph neural networks and variational approach to Markov processes for dynamical modeling of biomolecules. Journal of Chemical Physics, 2022, 156, 184103.	1.2	18
6	A reengineered common chain cytokine augments CD8+ T cellâ€“dependent immunotherapy. JCI Insight, 2022, 7, .	2.3	2
7	Computational Study of the Allosteric Effects of p5 on CDK5â€“p25 Hyperactivity as Alternative Inhibitory Mechanisms in Neurodegeneration. Journal of Physical Chemistry B, 2022, 126, 5033-5044.	1.2	2
8	CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. Journal of Chemical Theory and Computation, 2021, 17, 1581-1595.	2.3	45
9	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. Journal of Chemical Theory and Computation, 2021, 17, 1562-1580.	2.3	39
10	Location and Conformational Ensemble of Menaquinone and Menaquinol, and Proteinâ€“Lipid Modulations in Archaeal Membranes. Journal of Physical Chemistry B, 2021, 125, 4714-4725.	1.2	10
11	A replica exchange umbrella sampling (REUS) approach to predict hostâ€“guest binding free energies in SAMPL8 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 667-677.	1.3	5
12	Impact of PIP2 Lipids, Force Field Parameters, and Mutational Analysis on the Binding of the Osh4â€™s Î±₆â€“Î±₇ Domain. Journal of Physical Chemistry B, 2021, 125, 5296-5308.	1.2	1
13	Considerations of Recent All-Atom Lipid Force Field Development. Journal of Physical Chemistry B, 2021, 125, 5676-5682.	1.2	8
14	Estimating localization of various statins within a POPC bilayer. Chemistry and Physics of Lipids, 2021, 236, 105074.	1.5	7
15	Simulations of Diabetic and Non-Diabetic Peripheral Nerve Myelin Lipid Bilayers. Journal of Physical Chemistry B, 2021, 125, 6201-6213.	1.2	4
16	Virtual Issue on Docking. Journal of Physical Chemistry B, 2021, 125, 5455-5457.	1.2	0
17	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. Biophysical Journal, 2021, 120, 2902-2913.	0.2	22
18	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. Journal of Chemical Information and Modeling, 2021, 61, 831-839.	2.5	59

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19	Symmetric and Asymmetric Models for the Arabidopsis thaliana Plasma Membrane: A Simulation Study. Journal of Physical Chemistry B, 2021, 125, 11418-11431.	1.2	4
20	Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders. Journal of Chemical Physics, 2021, 155, 194108.	1.2	11
21	How Do Ethanolamine Plasmalogens Contribute to Order and Structure of Neurological Membranes?. Journal of Physical Chemistry B, 2020, 124, 828-839.	1.2	23
22	Microsecond-timescale simulations suggest 5-HTâ€“mediated preactivation of the 5-HT3Aserotonin receptor. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 405-414.	3.3	29
23	Molecular dynamics simulations of ethanol permeation through single and double-lipid bilayers. Journal of Chemical Physics, 2020, 153, 125101.	1.2	18
24	Critical Sequence Hotspots for Binding of Novel Coronavirus to Angiotensin Converter Enzyme as Evaluated by Molecular Simulations. Journal of Physical Chemistry B, 2020, 124, 10034-10047.	1.2	54
25	Membrane permeability of small molecules from unbiased molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 124107.	1.2	42
26	Interfacial properties of aqueous solutions of butanol isomers and cyclohexane. Fluid Phase Equilibria, 2020, 513, 112551.	1.4	4
27	Update of the CHARMM36 United Atom Chain Model for Hydrocarbons and Phospholipids. Journal of Physical Chemistry B, 2020, 124, 6797-6812.	1.2	16
28	Update of the CHARMM36 United Atom Chain Model for Lipids. Biophysical Journal, 2020, 118, 88a.	0.2	0
29	Investigation of Allosteric Inhibition Mechanisms by the Peptide p5 on the Alzheimer's Disease (AD) Pathological Complex cdk5-p25 through Molecular Dynamics Simulations. Biophysical Journal, 2020, 118, 206a.	0.2	0
30	Rapid, quantitative therapeutic screening for Alzheimer's enzymes enabled by optimal signal transduction with transistors. Analyst, The, 2020, 145, 2925-2936.	1.7	4
31	Modifying the CHARMM36 Lipid Force Field for LJ-PME Simulations. Biophysical Journal, 2020, 118, 87a.	0.2	1
32	Quantum capacitance-limited MoS₂biosensors enable remote label-free enzyme measurements. Nanoscale, 2019, 11, 15622-15632.	2.8	13
33	Probing the pH Effects on Sugar Binding to a Polysaccharide Lyase. Journal of Physical Chemistry B, 2019, 123, 7123-7136.	1.2	7
34	Molecular Structure of the Long Periodicity Phase in the Stratum Corneum. Journal of the American Chemical Society, 2019, 141, 16930-16943.	6.6	33
35	CHARMMâ€GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. Journal of Computational Chemistry, 2019, 40, 893-899.	1.5	42
36	Isothermal Titration Calorimetry of Be²⁺ with Phosphatidylserine Models Guides All-Atom Force-Field Development for Lipidâ€“Ion Interactions. Journal of Physical Chemistry B, 2019, 123, 1554-1565.	1.2	1

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37	Reproducible Performance Improvements to Monolayer MoS₂ Transistors through Exposed Material Forming Gas Annealing. ACS Applied Materials & Interfaces, 2019, 11, 16683-16692.	4.0	21
38	Physical Properties of Bacterial Outer Membrane Models: Neutron Reflectometry & Molecular Simulation. Biophysical Journal, 2019, 116, 1095-1104.	0.2	27
39	Mannobioseâ€Grafting Shifts PEI Charge and Biphasic Dependence on pH. Macromolecular Chemistry and Physics, 2019, 220, 1800423.	1.1	9
40	Structure and Permeability of Ceramide Bilayers and Multilayers. Journal of Physical Chemistry B, 2019, 123, 2525-2535.	1.2	19
41	Setting Up All-Atom Molecular Dynamics Simulations to Study the Interactions of Peripheral Membrane Proteins with Model Lipid Bilayers. Methods in Molecular Biology, 2019, 1949, 325-339.	0.4	8
42	Label-Free Enzyme Activity Measurements with Quantum-Limited Biosensors. Biophysical Journal, 2019, 116, 146a.	0.2	0
43	Developing and Testing of Lipid Force Fields with Applications to Modeling Cellular Membranes. Chemical Reviews, 2019, 119, 6227-6269.	23.0	72
44	Modeling Lipid Membranes. , 2019, , 741-759.		0
45	Effect of Membrane Lipid Packing on Stable Binding of the ALPS Peptide. Journal of Chemical Theory and Computation, 2019, 15, 1418-1429.	2.3	33
46	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. Journal of Chemical Theory and Computation, 2019, 15, 775-786.	2.3	388
47	Simulations of Pure Ceramide and Ternary Lipid Mixtures as Simple Interior Stratum Corneum Models. Journal of Physical Chemistry B, 2018, 122, 2757-2768.	1.2	33
48	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. Journal of Chemical Theory and Computation, 2018, 14, 948-958.	2.3	50
49	Investigation of phase transitions of saturated phosphocholine lipid bilayers via molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1489-1501.	1.4	57
50	Simulations of simple Bovine and Homo sapiens outer cortex ocular lens membrane models with a majority concentration of cholesterol. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2134-2144.	1.4	16
51	Engineering the Microbial Cell Membrane To Improve Bioproduction. ACS Symposium Series, 2018, , 25-39.	0.5	2
52	Modeling Pseudomonas aeruginosa inner plasma membrane in planktonic and biofilm modes. Journal of Chemical Physics, 2018, 149, 215102.	1.2	7
53	Perspective: Computational modeling of accurate cellular membranes with molecular resolution. Journal of Chemical Physics, 2018, 149, 220901.	1.2	17
54	Models for the Stratum Corneum Lipid Matrix: Effects of Ceramide Concentration, Ceramide Hydroxylation, and Free Fatty Acid Protonation. Journal of Physical Chemistry B, 2018, 122, 11996-12008.	1.2	18

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55	The Role of Lipid Interactions in Simulations of the Î±-Hemolysin Ion-Channel-Forming Toxin. Biophysical Journal, 2018, 115, 1720-1730.	0.2	10
56	Preferred Binding Mechanism of Osh4â€™s Amphipathic Lipid-Packing Sensor Motif, Insights from Molecular Dynamics. Journal of Physical Chemistry B, 2018, 122, 9713-9723.	1.2	18
57	Structural Events in a Bacterial Uniporter Leading to Translocation of Glucose to the Cytosol. Journal of Molecular Biology, 2018, 430, 3337-3352.	2.0	7
58	CHARMM-GUI Lecture Series on Molecular Modeling and Simulation. Biophysical Journal, 2018, 114, 184a.	0.2	0
59	Probing Plexin A3 Dimerization and the Importance of the Near Membrane Extracellular Residues. Biophysical Journal, 2018, 114, 423a.	0.2	0
60	Parameterization of the CHARMM All-Atom Force Field for Ether Lipids and Model Linear Ethers. Journal of Physical Chemistry B, 2018, 122, 6744-6754.	1.2	28
61	Aggregation of modified hexabenzocoronenes as models for early stage asphaltene self-assembly. Molecular Simulation, 2018, 44, 992-1003.	0.9	2
62	Examination of Mixtures Containing Sphingomyelin and Cholesterol by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 4833-4844.	1.2	40
63	Molecular Simulations of Mixed Lipid Bilayers with Sphingomyelin, Glycerophospholipids, and Cholesterol. Journal of Physical Chemistry B, 2017, 121, 5197-5208.	1.2	54
64	Simulations of simple linoleic acid-containing lipid membranes and models for the soybean plasma membranes. Journal of Chemical Physics, 2017, 146, 215103.	1.2	20
65	Analyzing the Effects of Lipid Type on the Î±-Hemolysin Nanopore andÂ5HT3 Receptor Structure and Gating using Molecular Dynamics Simulations. Biophysical Journal, 2017, 112, 275a-276a.	0.2	0
66	Simulation of Linoleoyl-Containing Pure Lipid Bilayer and Soybean Plasma Membranes. Biophysical Journal, 2017, 112, 82a.	0.2	1
67	Molecular Dynamics Simulations of Ceramide and Ceramide-Phosphatidylcholine Bilayers. Journal of Physical Chemistry B, 2017, 121, 10091-10104.	1.2	26
68	Engineering Escherichia coli membrane phospholipid head distribution improves tolerance and production of biorenewables. Metabolic Engineering, 2017, 44, 1-12.	3.6	83
69	Two sterols, two bilayers: insights on membrane structure from molecular dynamics. Molecular Simulation, 2017, 43, 1179-1188.	0.9	10
70	Dual Action of Hydrotropes at the Water/Oil Interface. Journal of Physical Chemistry C, 2017, 121, 16423-16431.	1.5	24
71	CHARMM-GUI Input Generator for NAMD, Gromacs, Amber, Openmm, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. Biophysical Journal, 2016, 110, 641a.	0.2	63
72	Effects of Spin-Labels on Membrane Burial Depth of MARCKS-ED Residues. Biophysical Journal, 2016, 111, 1600-1603.	0.2	0

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73	Water Orientation at Ceramide/Water Interfaces Studied by Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2016, 120, 23692-23697.	1.5	12
74	Interplay of Specific Trans- and Juxtamembrane Interfaces in Plexin A3 Dimerization and Signal Transduction. Biochemistry, 2016, 55, 4928-4938.	1.2	5
75	An extensive simulation study of lipid bilayer properties with different head groups, acyl chain lengths, and chain saturations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 3093-3104.	1.4	51
76	Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. Journal of Physical Chemistry B, 2016, 120, 11761-11772.	1.2	47
77	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. Biophysical Journal, 2016, 111, 1750-1760.	0.2	88
78	Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. Biophysical Journal, 2016, 111, 1987-1999.	0.2	41
79	Modeling structural transitions from the periplasmic-open state of lactose permease and interpretations of spin label experiments. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1541-1552.	1.4	5
80	Probing the Ripple Phase of Lipid Bilayers using Molecular Simulations. Biophysical Journal, 2016, 110, 86a.	0.2	2
81	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2016, 12, 405-413.	2.3	2,567
82	The simultaneous mass and energy evaporation (SM2E) model. Journal of Occupational and Environmental Hygiene, 2016, 13, 243-253.	0.4	1
83	Peripheral membrane proteins: Tying the knot between experiment and computation. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1584-1593.	1.4	48
84	Modeling Lipid Membranes. , 2016, , 1-19.		0
85	Molecular dynamics simulations of cholesterol-rich membranes using a coarse-grained force field for cyclic alkanes. Journal of Chemical Physics, 2015, 143, 243144.	1.2	55
86	How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets?. Journal of Chemical Theory and Computation, 2015, 11, 3466-3477.	2.3	64
87	Molecular Dynamics Simulations on the Periplasmic-Open State Lactose Permease. Biophysical Journal, 2015, 108, 466a.	0.2	0
88	Biophysical Changes of Lipid Membranes in the Presence of Ethanol at Varying Concentrations. Journal of Physical Chemistry B, 2015, 119, 13134-13141.	1.2	27
89	Modeling Yeast Organelle Membranes and How Lipid Diversity Influences Bilayer Properties. Biochemistry, 2015, 54, 6852-6861.	1.2	58
90	Probing the importance of lipid diversity in cell membranes via molecular simulation. Chemistry and Physics of Lipids, 2015, 192, 12-22.	1.5	56

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91	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. Biophysical Journal, 2015, 109, 2012-2022.	0.2	89
92	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. Biophysical Journal, 2015, 109, 2090-2100.	0.2	18
93	Molecular dynamics simulations of palmitoyloleoylphosphatidylglycerol bilayers. Molecular Simulation, 2015, 41, 948-954.	0.9	9
94	Lipopolysaccharide Membrane Building and Simulation. Methods in Molecular Biology, 2015, 1273, 391-406.	0.4	41
95	STâ€analyzer: A webâ€based user interface for simulation trajectory analysis. Journal of Computational Chemistry, 2014, 35, 957-963.	1.5	12
96	Lipid-Linked Oligosaccharides in Membranes Sample Conformations That Facilitate Binding to Oligosaccharyltransferase. Biophysical Journal, 2014, 107, 1885-1895.	0.2	21
97	CHARMM-GUIMembrane Buildertoward realistic biological membrane simulations. Journal of Computational Chemistry, 2014, 35, 1997-2004.	1.5	1,802
98	Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms. Journal of Physical Chemistry B, 2014, 118, 4315-4325.	1.2	38
99	A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2520-2529.	1.4	82
100	CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature. Biophysical Journal, 2014, 107, 134-145.	0.2	192
101	CHARMM36 United Atom Chain Model for Lipids and Surfactants. Journal of Physical Chemistry B, 2014, 118, 547-556.	1.2	143
102	Mesoscale Phenomena in Ternary Solutions of Tertiary Butyl Alcohol, Water, and Propylene Oxide. Journal of Physical Chemistry B, 2014, 118, 5994-6006.	1.2	39
103	E.Âcoli Outer Membrane and Interactions with OmpLA. Biophysical Journal, 2014, 106, 2493-2502.	0.2	128
104	Mesoscale inhomogeneities in aqueous solutions of small amphiphilic molecules. Faraday Discussions, 2013, 167, 217.	1.6	86
105	Molecular Dynamics and NMR Spectroscopy Studies of E.Âcoli Lipopolysaccharide Structure and Dynamics. Biophysical Journal, 2013, 105, 1444-1455.	0.2	153
106	CHARMM-GUI Micelle Builder for Pure/Mixed Micelle and Protein/Micelle Complex Systems. Journal of Chemical Information and Modeling, 2013, 53, 2171-2180.	2.5	99
107	Influence of Ester-Modified Lipids on Bilayer Structure. Langmuir, 2013, 29, 14196-14203.	1.6	15
108	Developing CHARMM-Compatible Lipid Parameters for Ceramides and United Atom Chains. Biophysical Journal, 2013, 104, 591a.	0.2	1

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109	Molecular Dynamics Simulations of the Cx26 Hemichannel: Insights into Voltage-Dependent Loop-Gating. Biophysical Journal, 2012, 102, 1341-1351.	0.2	35
110	Membrane models of E. coli containing cyclic moieties in the aliphatic lipid chain. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 1205-1210.	1.4	89
111	Improving the CHARMM Force Field for Polyunsaturated Fatty Acid Chains. Journal of Physical Chemistry B, 2012, 116, 9424-9431.	1.2	140
112	Membrane-Binding Mechanism of a Peripheral Membrane Protein through Microsecond Molecular Dynamics Simulations. Journal of Molecular Biology, 2012, 423, 847-861.	2.0	41
113	Update of the Cholesterol Force Field Parameters in CHARMM. Journal of Physical Chemistry B, 2012, 116, 203-210.	1.2	185
114	Lipid Membranes with a Majority of Cholesterol: Applications to the Ocular Lens and Aquaporin 0. Journal of Physical Chemistry B, 2011, 115, 6455-6464.	1.2	44
115	Orientation of Fluorescent Lipid Analogue BODIPY-PC to Probe Lipid Membrane Properties: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 6157-6165.	1.2	26
116	Gas Hydrate Structure and Pressure Predictions Based on an Updated Fugacity-Based Model with the PSRK Equation of State. Industrial & Engineering Chemistry Research, 2011, 50, 148-157.	1.8	36
117	Lipid chain branching at the iso- and anteiso-positions in complex chlamydia membranes: A molecular dynamics study. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 323-331.	1.4	49
118	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. Journal of Physical Chemistry B, 2010, 114, 7830-7843.	1.2	3,676
119	Cholesterol Flip-Flop: Insights from Free Energy Simulation Studies. Journal of Physical Chemistry B, 2010, 114, 13342-13348.	1.2	109
120	Sterol Binding and Membrane Lipid Attachment to the Osh4 Protein of Yeast. Journal of Physical Chemistry B, 2010, 114, 13562-13573.	1.2	5
121	Probing the Periplasmic-Open State of Lactose Permease in Response to Sugar Binding and Proton Translocation. Journal of Molecular Biology, 2010, 404, 506-521.	2.0	30
122	Binding of A Natural Sterol to the Osh4 Protein of Yeast and Membrane Attachment. Biophysical Journal, 2010, 98, 241a.	0.2	0
123	A Modified Lipid Force Field for Charmm: Development and Application to Single-Celled Organism Membranes. Biophysical Journal, 2010, 98, 282a.	0.2	0
124	Binding and release of cholesterol in the Osh4 protein of yeast. Proteins: Structure, Function and Bioinformatics, 2009, 75, 468-477.	1.5	33
125	CHARMM-GUI Membrane Builder for Mixed Bilayers and Its Application to Yeast Membranes. Biophysical Journal, 2009, 97, 50-58.	0.2	1,346
126	Chapter 1 Considerations for Lipid Force Field Development. Current Topics in Membranes, 2008, , 1-48.	0.5	54

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127	Rotation of Lipids in Membranes: Molecular Dynamics Simulation, 31P Spin-Lattice Relaxation, and Rigid-Body Dynamics. Biophysical Journal, 2008, 94, 3074-3083.	0.2	94
128	Collective and Noncollective Models of NMR Relaxation in Lipid Vesicles and Multilayers. Journal of Physical Chemistry B, 2008, 112, 5924-5929.	1.2	53
129	CHARMMing: A New, Flexible Web Portal for CHARMM. Journal of Chemical Information and Modeling, 2008, 48, 1920-1929.	2.5	118
130	CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. Journal of Chemical Theory and Computation, 2008, 4, 107-115.	2.3	11
131	Sugar Binding in Lactose Permease: Anomeric State of a Disaccharide Influences Binding Structure. Journal of Molecular Biology, 2007, 367, 1523-1534.	2.0	30
132	Long-Range Lennard-Jones and Electrostatic Interactions in Interfaces:Â Application of the Isotropic Periodic Sum Method. Journal of Physical Chemistry B, 2007, 111, 4393-4400.	1.2	78
133	Dynamical motions of lipids and a finite size effect in simulations of bilayers. Journal of Chemical Physics, 2006, 125, 144710.	1.2	117
134	Simulation-Based Methods for Interpreting X-Ray Data from Lipid Bilayers. Biophysical Journal, 2006, 90, 2796-2807.	0.2	219
135	Hierarchical Modeling N2Adsorption on the Surface of and within a C60Crystal:Â From Quantum Mechanics to Molecular Simulation. Journal of Physical Chemistry B, 2005, 109, 4731-4737.	1.2	13
136	Adjacent Gauche Stabilization in Linear Alkanes:Â Implications for Polymer Models and Conformational Analysis. Journal of Physical Chemistry B, 2005, 109, 15684-15686.	1.2	53
137	A Comparative Study of Nitrogen Physisorption on Different C70Crystal Structures Using an Ab Initio Based Potential. Journal of Physical Chemistry B, 2005, 109, 17267-17273.	1.2	4
138	Global Distribution of Methane Hydrate in Ocean Sediment. Energy & Fuels, 2005, 19, 459-470.	2.5	459
139	An ab Initio Study on the Torsional Surface of Alkanes and Its Effect on Molecular Simulations of Alkanes and a DPPC Bilayer. Journal of Physical Chemistry B, 2005, 109, 5300-5311.	1.2	303
140	HM-IE:â€‰ Quantum Chemical Hybrid Methods for Calculating Interaction Energies. Journal of Physical Chemistry A, 2004, 108, 107-112.	1.1	44
141	Hierarchical Modeling O2 and N2 Adsorption in C168 Schwarzite:â€‰ From Quantum Mechanics to Molecular Simulation. Journal of Physical Chemistry B, 2004, 108, 9852-9860.	1.2	16
142	An ab Initio Study on the Effect of Carbon Surface Curvature and Ring Structure on N2(O2)â^'Carbon Intermolecular Potentials. Journal of Physical Chemistry B, 2004, 108, 9842-9851.	1.2	30
143	Phase behavior of clathrate hydrates: a model for single and multiple gas component hydrates. Chemical Engineering Science, 2003, 58, 27-41.	1.9	168
144	Monte Carlo Simulation of O2and N2Adsorption in Nanoporous Carbon (C168Schwarzite). Langmuir, 2003, 19, 3512-3518.	1.6	32

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145	Predictions of gas hydrate phase equilibria and amounts in natural sediment porous media. Marine and Petroleum Geology, 2003, 20, 459-470.	1.5	67
146	Ab Initio Intermolecular Potentials for Gas Hydrates and Their Predictions. Journal of Physical Chemistry B, 2002, 106, 5722-5732.	1.2	80
147	Modeling Gas Hydrate Phase Equilibria in Laboratory and Natural Porous Media. Industrial & Engineering Chemistry Research, 2001, 40, 4197-4208.	1.8	91
148	A Fugacity Model for Gas Hydrate Phase Equilibria. Industrial & Engineering Chemistry Research, 2000, 39, 3377-3386.	1.8	246