

Sandeep Patel

List of Publications by Year in descending order

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63
papers

2,965
citations

185998

28
h-index

161609

54
g-index

64
all docs

64
docs citations

64
times ranked

2753
citing authors

#	ARTICLE	IF	CITATIONS
1	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. <i>Journal of Computational Chemistry</i> , 2004, 25, 1-16.	1.5	457
2	CHARMM fluctuating charge force field for proteins: II Protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model. <i>Journal of Computational Chemistry</i> , 2004, 25, 1504-1514.	1.5	410
3	Chemical and electrochemical copolymerization of aniline with alkyl ring-substituted anilines. <i>Macromolecules</i> , 1990, 23, 758-764.	2.2	257
4	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. <i>Molecular Simulation</i> , 2006, 32, 231-249.	0.9	116
5	Hydration free energies of monovalent ions in transferable intermolecular potential four point fluctuating charge water: An assessment of simulation methodology and force field performance and transferability. <i>Journal of Chemical Physics</i> , 2007, 127, 064509.	1.2	107
6	Origin and control of superlinear polarizability scaling in chemical potential equalization methods. <i>Journal of Chemical Physics</i> , 2008, 128, 144110.	1.2	77
7	Insights into Thiol-Aromatic Interactions: A Stereoelectronic Basis for S-H Interactions. <i>Journal of the American Chemical Society</i> , 2017, 139, 1842-1855.	6.6	76
8	Thermodynamic and structural properties of methanol-water solutions using nonadditive interaction models. <i>Journal of Computational Chemistry</i> , 2008, 29, 1142-1152.	1.5	73
9	A nonadditive methanol force field: Bulk liquid and liquid-vapor interfacial properties via molecular dynamics simulations using a fluctuating charge model. <i>Journal of Chemical Physics</i> , 2005, 122, 024508.	1.2	66
10	Structure, thermodynamics, and liquid-vapor equilibrium of ethanol from molecular-dynamics simulations using nonadditive interactions. <i>Journal of Chemical Physics</i> , 2005, 123, 164502.	1.2	63
11	Revisiting the hexane-water interface via molecular dynamics simulations using nonadditive alkane-water potentials. <i>Journal of Chemical Physics</i> , 2006, 124, 204706.	1.2	58
12	Exploring Ion Permeation Energetics in Gramicidin A Using Polarizable Charge Equilibration Force Fields. <i>Journal of the American Chemical Society</i> , 2009, 131, 13890-13891.	6.6	58
13	Molecular Dynamics Simulations of a DMPC Bilayer Using Nonadditive Interaction Models. <i>Biophysical Journal</i> , 2009, 96, 385-402.	0.2	55
14	Investigating Hydrophilic Pores in Model Lipid Bilayers Using Molecular Simulations: Correlating Bilayer Properties with Pore-Formation Thermodynamics. <i>Langmuir</i> , 2015, 31, 6615-6631.	1.6	54
15	Comparison of the Solvation Structure of Polarizable and Nonpolarizable Ions in Bulk Water and Near the Aqueous Liquid-Vapor Interface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 7455-7467.	1.5	52
16	Free Energetics of Arginine Permeation into Model DMPC Lipid Bilayers: Coupling of Effective Counterion Concentration and Lateral Bilayer Dimensions. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11641-11653.	1.2	48
17	Charge Equilibration Force Fields for Lipid Environments: Applications to Fully Hydrated DPPC Bilayers and DMPC-Embedded Gramicidin A. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9183-9196.	1.2	46
18	Nonadditive Empirical Force Fields for Short-Chain Linear Alcohols: Methanol to Butanol. Hydration Free Energetics and Kirkwood-Buffer Analysis Using Charge Equilibration Models. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11076-11092.	1.2	45

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19	Recent applications and developments of charge equilibration force fields for modeling dynamical charges in classical molecular dynamics simulations. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	41
20	Electrostatic Properties of Aqueous Salt Solution Interfaces: A Comparison of Polarizable and Nonpolarizable Ion Models. <i>Journal of Physical Chemistry B</i> , 2008, 112, 11679-11693.	1.2	40
21	Properties of water along the liquid-vapor coexistence curve via molecular dynamics simulations using the polarizable TIP4P-QDP-LJ water model. <i>Journal of Chemical Physics</i> , 2009, 131, 084709.	1.2	40
22	Improving numerical reproducibility and stability in large-scale numerical simulations on GPUs. , 2010, , .		38
23	Revised Charge Equilibration Potential for Liquid Alkanes. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8298-8310.	1.2	36
24	Charge equilibration force fields for molecular dynamics simulations of lipids, bilayers, and integral membrane protein systems. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 318-329.	1.4	36
25	Incorporating Phase-Dependent Polarizability in Nonadditive Electrostatic Models for Molecular Dynamics Simulations of the Aqueous Liquid-Vapor Interface. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 359-373.	2.3	33
26	Electrostatic Polarization Effects and Hydrophobic Hydration in Ethanol-Water Solutions from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 767-778.	1.2	31
27	Translocation Thermodynamics of Linear and Cyclic Nonaarginine into Model DPPC Bilayer via Coarse-Grained Molecular Dynamics Simulation: Implications of Pore Formation and Nonadditivity. <i>Journal of Physical Chemistry B</i> , 2014, 118, 2670-2682.	1.2	31
28	Water permeation through DMPC lipid bilayers using polarizable charge equilibration force fields. <i>Chemical Physics Letters</i> , 2011, 508, 289-294.	1.2	29
29	Molecular dynamics simulations of aqueous ions at the liquid-vapor interface accelerated using graphics processors. <i>Journal of Computational Chemistry</i> , 2011, 32, 375-385.	1.5	28
30	Thermodynamics of cell-penetrating HIV1 TAT peptide insertion into PC/PS/CHOL model bilayers through transmembrane pores: the roles of cholesterol and anionic lipids. <i>Soft Matter</i> , 2016, 12, 6716-6727.	1.2	28
31	Free Energetics of Carbon Nanotube Association in Pure and Aqueous Ionic Solutions. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8154-8168.	1.2	27
32	Solvation properties of N-acetylglucosamine: Molecular dynamics study incorporating electrostatic polarization. <i>Journal of Computational Chemistry</i> , 2011, 32, 3339-3353.	1.5	24
33	Variation of Ion Polarizability from Vacuum to Hydration: Insights from Hirshfeld Partitioning. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8984-8992.	1.1	23
34	Free Energetics and the Role of Water in the Permeation of Methyl Guanidinium across the Bilayer-Water Interface: Insights from Molecular Dynamics Simulations Using Charge Equilibration Potentials. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3578-3592.	1.2	23
35	Structural, dynamic, and electrostatic properties of fully hydrated DMPC bilayers from molecular dynamics simulations accelerated with graphical processing units (GPUs). <i>Journal of Computational Chemistry</i> , 2011, 32, 2958-2973.	1.5	22
36	Temperature Dependence and Energetics of Single Ions at the Aqueous Liquid-Vapor Interface. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6512-6523.	1.2	22

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37	Condensed-phase properties of n-alkyl-amines from molecular dynamics simulations using charge equilibration force fields. <i>Journal of Molecular Liquids</i> , 2008, 142, 32-40.	2.3	19
38	Interfacial Structure, Thermodynamics, and Electrostatics of Aqueous Methanol Solutions via Molecular Dynamics Simulations Using Charge Equilibration Models. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9241-9254.	1.2	19
39	Binding structures of tri- <i>N</i> -acetyl- β -glucosamine in hen egg white lysozyme using molecular dynamics with a polarizable force field. <i>Journal of Computational Chemistry</i> , 2013, 34, 163-174.	1.5	19
40	Spherical Monovalent Ions at Aqueous Liquid-Vapor Interfaces: Interfacial Stability and Induced Interface Fluctuations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11732-11742.	1.2	19
41	Protein Denaturants at Aqueous Hydrophobic Interfaces: Self-Consistent Correlation between Induced Interfacial Fluctuations and Denaturant Stability at the Interface. <i>Journal of Physical Chemistry B</i> , 2015, 119, 164-178.	1.2	18
42	Solvation structure and energetics of single ions at the aqueous liquid-vapor interface. <i>Chemical Physics Letters</i> , 2012, 527, 22-26.	1.2	16
43	Molecular dynamics simulation of hydrated DPPC monolayers using charge equilibration force fields. <i>Journal of Computational Chemistry</i> , 2012, 33, 141-152.	1.5	16
44	Dynamics and energetics of hydrophobically confined water. <i>Physical Review E</i> , 2012, 85, 051506.	0.8	15
45	Role of Electrostatics in Modulating Hydrophobic Interactions and Barriers to Hydrophobic Assembly. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8107-8117.	1.2	14
46	GPU-Enabled Macromolecular Simulation: Challenges and Opportunities. <i>Computing in Science and Engineering</i> , 2013, 15, 56-65.	1.2	14
47	Reconciling Structural and Thermodynamic Predictions Using All-Atom and Coarse-Grain Force Fields: The Case of Charged Oligo-Arginine Translocation into DMPC Bilayers. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11973-11992.	1.2	14
48	Molecular dynamics simulations of nonpolarizable inorganic salt solution interfaces: NaCl, NaBr, and NaI in transferable intermolecular potential 4-point with charge dependent polarizability (TIP4P-QDP) water. <i>Journal of Chemical Physics</i> , 2010, 132, 024713.	1.2	13
49	Liquid-Vapor Interfacial Properties of Aqueous Solutions of Guanidinium and Methyl Guanidinium Chloride: Influence of Molecular Orientation on Interface Fluctuations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11719-11731.	1.2	13
50	Ion-Specific Induced Fluctuations and Free Energetics of Aqueous Protein Hydrophobic Interfaces: Toward Connecting to Specific-Ion Behaviors at Aqueous Liquid-Vapor Interfaces. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4490-4504.	1.2	12
51	Role of spatial ionic distribution on the energetics of hydrophobic assembly and properties of the water/hydrophobe interface. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1892.	1.3	11
52	Revised charge equilibration parameters for more accurate hydration free energies of alkanes. <i>Chemical Physics Letters</i> , 2010, 484, 173-176.	1.2	10
53	FENZI: GPU-Enabled Molecular Dynamics Simulations of Large Membrane Regions Based on the CHARMM Force Field and PME. , 2011, , .		10
54	Phase-transfer energetics of small-molecule alcohols across the water-hexane interface: Molecular dynamics simulations using charge equilibration models. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 29, 876-887.	1.3	10

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55	Free energetics of rigid body association of ubiquitin binding domains: A biochemical model for binding mediated by hydrophobic interaction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1453-1468.	1.5	9
56	A charge equilibration formalism for treating charge transfer effects in MD simulations: Application to water clusters. <i>Journal of Computational Chemistry</i> , 2017, 38, 1389-1409.	1.5	8
57	Molecular modeling of ions at interfaces: exploring similarities to hydrophobic solvation through the lens of induced aqueous interfacial fluctuations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30357-30365.	1.3	7
58	Association of alkanes with the aqueous liquid-vapor interface: a reference system for interpreting hydrophobicity generally through interfacial fluctuations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26779-26785.	1.3	3
59	Electrostatic contribution from solvent in modulating single-walled carbon nanotube association. <i>Journal of Chemical Physics</i> , 2014, 141, 114906.	1.2	2
60	Pursuing Coordinated Trajectory Progression and Efficient Resource Utilization of GPU-Enabled Molecular Dynamics Simulations. <i>IEEE Design and Test</i> , 2014, 31, 40-50.	1.1	2
61	Free energetics of carbon nanotube association in aqueous inorganic NaCl salt solutions: Temperature effects using all-atom molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2015, 36, 1196-1212.	1.5	2
62	Exploring Protein-Ligand Binding using Charge Equilibration Force Fields. <i>Biophysical Journal</i> , 2011, 100, 393a.	0.2	0
63	Efficient SDS Simulations on Multi-GPU Nodes of XSEDE High-End Clusters. , 2013, , .		0