Sandeep Patel

List of Publications by Year
in descending order

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63	2,965	186265	161849
papers	citations	28 h-index	54 g-index

64	64	64	2753
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. Journal of Computational Chemistry, 2004, 25, 1-16.	3.3	457
2	CHARMM fluctuating charge force field for proteins: II Protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model. Journal of Computational Chemistry, 2004, 25, 1504-1514.	3.3	410
3	Chemical and electrochemical copolymerization of aniline with alkyl ring-substituted anilines. Macromolecules, 1990, 23, 758-764.	4.8	257
4	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. Molecular Simulation, 2006, 32, 231-249.	2.0	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. Journal of Chemical Physics, 2007, 127, 064509.	3.0	107
6	Origin and control of superlinear polarizability scaling in chemical potential equalization methods. Journal of Chemical Physics, 2008, 128, 144110.	3.0	77
7	Insights into Thiolâ€“Aromatic Interactions: A Stereoelectronic Basis for Sâ€“H/Ï€ Interactions. Journal of the American Chemical Society, 2017, 139, 1842-1855.	13.7	76
8	Thermodynamic and structural properties of methanolâ€“water solutions using nonadditive interaction models. Journal of Computational Chemistry, 2008, 29, 1142-1152.	3.3	73
9	A nonadditive methanol force field: Bulk liquid and liquid-vapor interfacial properties via molecular dynamics simulations using a fluctuating charge model. Journal of Chemical Physics, 2005, 122, 024508.	3.0	66
10	Structure, thermodynamics, and liquid-vapor equilibrium of ethanol from molecular-dynamics simulations using nonadditive interactions. Journal of Chemical Physics, 2005, 123, 164502.	3.0	63
11	Revisiting the hexane-water interface via molecular dynamics simulations using nonadditive alkane-water potentials. Journal of Chemical Physics, 2006, 124, 204706.	3.0	58
12	Exploring Ion Permeation Energetics in Gramicidin A Using Polarizable Charge Equilibration Force Fields. Journal of the American Chemical Society, 2009, 131, 13890-13891.	13.7	58
13	Molecular Dynamics Simulations of a DMPC Bilayer Using Nonadditive Interaction Models. Biophysical Journal, 2009, 96, 385-402.	0.5	55
14	Investigating Hydrophilic Pores in Model Lipid Bilayers Using Molecular Simulations: Correlating Bilayer Properties with Pore-Formation Thermodynamics. Langmuir, 2015, 31, 6615-6631.	3.5	54
15	Comparison of the Solvation Structure of Polarizable and Nonpolarizable Ions in Bulk Water and Near the Aqueous Liquidâ^'Vapor Interface. Journal of Physical Chemistry C, 2008, 112, 7455-7467.	3.1	52
16	Free Energetics of Arginine Permeation into Model DMPC Lipid Bilayers: Coupling of Effective Counterion Concentration and Lateral Bilayer Dimensions. Journal of Physical Chemistry B, 2013, 117, 11641-11653.	2.6	48
17	Charge Equilibration Force Fields for Lipid Environments: Applications to Fully Hydrated DPPC Bilayers and DMPC-Embedded Gramicidin A. Journal of Physical Chemistry B, 2009, 113, 9183-9196.	2.6	46
18	Nonadditive Empirical Force Fields for Short-Chain Linear Alcohols: Methanol to Butanol. Hydration Free Energetics and Kirkwoodâ^'Buff Analysis Using Charge Equilibration Models. Journal of Physical Chemistry B, 2010, 114, 11076-11092.	2.6	45

#	Article	IF	Citations
19	Recent applications and developments of charge equilibration force fields for modeling dynamical charges in classical molecular dynamics simulations. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	41
20	Electrostatic Properties of Aqueous Salt Solution Interfaces: A Comparison of Polarizable and Nonpolarizable Ion Models. Journal of Physical Chemistry B, 2008, 112, 11679-11693.	2.6	40
21	Properties of water along the liquid-vapor coexistence curve via molecular dynamics simulations using the polarizable TIP4P-QDP-LJ water model. Journal of Chemical Physics, 2009, 131, 084709.	3.0	40
22	Improving numerical reproducibility and stability in large-scale numerical simulations on GPUs. , 2010, , .		38
23	Revised Charge Equilibration Potential for Liquid Alkanes. Journal of Physical Chemistry B, 2008, 112, 8298-8310.	2.6	36
24	Charge equilibration force fields for molecular dynamics simulations of lipids, bilayers, and integral membrane protein systems. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 318-329.	2.6	36
25	Incorporating Phase-Dependent Polarizability in Nonadditive Electrostatic Models for Molecular Dynamics Simulations of the Aqueous Liquidâ^'Vapor Interface. Journal of Chemical Theory and Computation, 2009, 5, 359-373.	5.3	33
26	Electrostatic Polarization Effects and Hydrophobic Hydration in Ethanolâ^'Water Solutions from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 767-778.	2.6	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. Journal of Physical Chemistry B, 2014, 118, 2670-2682.	2.6	31
28	Water permeation through DMPC lipid bilayers using polarizable charge equilibration force fields. Chemical Physics Letters, 2011, 508, 289-294.	2.6	29
29	Molecular dynamics simulations of aqueous ions at the liquidâ€"vapor interface accelerated using graphics processors. Journal of Computational Chemistry, 2011, 32, 375-385.	3.3	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. Soft Matter, 2016, 12, 6716-6727.	2.7	28
31	Free Energetics of Carbon Nanotube Association in Pure and Aqueous Ionic Solutions. Journal of Physical Chemistry B, 2012, 116, 8154-8168.	2.6	27
32	Solvation properties of Nâ€acetylâ€Î²â€glucosamine: Molecular dynamics study incorporating electrostatic polarization. Journal of Computational Chemistry, 2011, 32, 3339-3353.	3.3	24
33	Variation of Ion Polarizability from Vacuum to Hydration: Insights from Hirshfeld Partitioning. Journal of Physical Chemistry A, 2010, 114, 8984-8992.	2.5	23
34	Free Energetics and the Role of Water in the Permeation of Methyl Guanidinium across the Bilayerâ€"Water Interface: Insights from Molecular Dynamics Simulations Using Charge Equilibration Potentials. Journal of Physical Chemistry B, 2013, 117, 3578-3592.	2.6	23
35	Structural, dynamic, and electrostatic properties of fully hydrated DMPC bilayers from molecular dynamics simulations accelerated with graphical processing units (GPUs). Journal of Computational Chemistry, 2011, 32, 2958-2973.	3.3	22
36	Temperature Dependence and Energetics of Single Ions at the Aqueous Liquidâ€"Vapor Interface. Journal of Physical Chemistry B, 2013, 117, 6512-6523.	2.6	22

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37	Condensed-phase properties of n-alkyl-amines from molecular dynamics simulations using charge equilibration force fields. Journal of Molecular Liquids, 2008, 142, 32-40.	4.9	19
38	Interfacial Structure, Thermodynamics, and Electrostatics of Aqueous Methanol Solutions via Molecular Dynamics Simulations Using Charge Equilibration Models. Journal of Physical Chemistry B, 2009, 113, 9241-9254.	2.6	19
39	Binding structures of triâ€Nâ€acetylâ€Î²â€glucosamine in hen egg white lysozyme using molecular dynamics with a polarizable force field. Journal of Computational Chemistry, 2013, 34, 163-174.	3.3	19
40	Spherical Monovalent Ions at Aqueous Liquidâ€“Vapor Interfaces: Interfacial Stability and Induced Interface Fluctuations. Journal of Physical Chemistry B, 2013, 117, 11732-11742.	2.6	19
41	Protein Denaturants at Aqueousâ€“Hydrophobic Interfaces: Self-Consistent Correlation between Induced Interfacial Fluctuations and Denaturant Stability at the Interface. Journal of Physical Chemistry B, 2015, 119, 164-178.	2.6	18
42	Solvation structure and energetics of single ions at the aqueous liquidâ€“vapor interface. Chemical Physics Letters, 2012, 527, 22-26.	2.6	16
43	Molecular dynamics simulation of hydrated DPPC monolayers using charge equilibration force fields. Journal of Computational Chemistry, 2012, 33, 141-152.	3.3	16
44	Dynamics and energetics of hydrophobically confined water. Physical Review E, 2012, 85, 051506.	2.1	15
45	Role of Electrostatics in Modulating Hydrophobic Interactions and Barriers to Hydrophobic Assembly. Journal of Physical Chemistry B, 2010, 114, 8107-8117.	2.6	14
46	GPU-Enabled Macromolecular Simulation: Challenges and Opportunities. Computing in Science and Engineering, 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. Journal of Physical Chemistry B, 2014, 118, 11973-11992.	2.6	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. Journal of Chemical Physics, 2010, 132, 024713.	3.0	13
49	Liquidâ€“Vapor Interfacial Properties of Aqueous Solutions of Guanidinium and Methyl Guanidinium Chloride: Influence of Molecular Orientation on Interface Fluctuations. Journal of Physical Chemistry B, 2013, 117, 11719-11731.	2.6	13
50	Ion-Specific Induced Fluctuations and Free Energetics of Aqueous Protein Hydrophobic Interfaces: Toward Connecting to Specific-Ion Behaviors at Aqueous Liquidâ€“Vapor Interfaces. Journal of Physical Chemistry B, 2014, 118, 4490-4504.	2.6	12
51	Role of spatial ionic distribution on the energetics of hydrophobic assembly and properties of the water/hydrophobe interface. Physical Chemistry Chemical Physics, 2012, 14, 1892.	2.8	11
52	Revised charge equilibration parameters for more accurate hydration free energies of alkanes. Chemical Physics Letters, 2010, 484, 173-176.	2.6	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 waterâ€“hexane interface: Molecular dynamics simulations using charge equilibration models. Journal of Molecular Graphics and Modelling, 2011, 29, 876-887.	2.4	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. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1453-1468.	2.6	9
56	A charge equilibration formalism for treating charge transfer effects in MD simulations: Application to water clusters. Journal of Computational Chemistry, 2017, 38, 1389-1409.	3.3	8
57	Molecular modeling of ions at interfaces: exploring similarities to hydrophobic solvation through the lens of induced aqueous interfacial fluctuations. Physical Chemistry Chemical Physics, 2016, 18, 30357-30365.	2.8	7
58	Association of alkanes with the aqueous liquidâ€“vapor interface: a reference system for interpreting hydrophobicity generally through interfacial fluctuations. Physical Chemistry Chemical Physics, 2014, 16, 26779-26785.	2.8	3
59	Electrostatic contribution from solvent in modulating single-walled carbon nanotube association. Journal of Chemical Physics, 2014, 141, 114906.	3.0	2
60	Pursuing Coordinated Trajectory Progression and Efficient Resource Utilization of GPU-Enabled Molecular Dynamics Simulations. IEEE Design and Test, 2014, 31, 40-50.	1.2	2
61	Free energetics of carbon nanotube association in aqueous inorganic <scp>N</scp>a<scp>I</scp> salt solutions: Temperature effects using allâ€atom molecular dynamics simulations. Journal of Computational Chemistry, 2015, 36, 1196-1212.	3.3	2
62	Exploring Protein-Ligand Binding using Charge Equilibration Force Fields. Biophysical Journal, 2011, 100, 393a.	0.5	0
63	Efficient SDS Simulations on Multi-GPU Nodes of XSEDE High-End Clusters. , 2013, , .		0