

Sandeep Patel

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62
papers

2,630
citations

26
h-index

50
g-index

64
ext. papers

2,807
ext. citations

3.7
avg, IF

5.28
L-index

#	Paper	IF	Citations
62	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1-15	3.5	414
61	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, 1504-14	3.5	371
60	Chemical and electrochemical copolymerization of aniline with alkyl ring-substituted anilines. <i>Macromolecules</i> , 1990 , 23, 758-764	5.5	235
59	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. <i>Molecular Simulation</i> , 2006 , 32, 231-249	2	101
58	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	3.9	97
57	Origin and control of superlinear polarizability scaling in chemical potential equalization methods. <i>Journal of Chemical Physics</i> , 2008 , 128, 144110	3.9	67
56	Thermodynamic and structural properties of methanol-water solutions using nonadditive interaction models. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1142-52	3.5	61
55	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	3.9	61
54	Structure, thermodynamics, and liquid-vapor equilibrium of ethanol from molecular-dynamics simulations using nonadditive interactions. <i>Journal of Chemical Physics</i> , 2005 , 123, 164502	3.9	58
53	Insights into Thiol-Aromatic Interactions: A Stereoelectronic Basis for S-H/π Interactions. <i>Journal of the American Chemical Society</i> , 2017 , 139, 1842-1855	16.4	54
52	Revisiting the hexane-water interface via molecular dynamics simulations using nonadditive alkane-water potentials. <i>Journal of Chemical Physics</i> , 2006 , 124, 204706	3.9	54
51	Molecular dynamics simulations of a DMPC bilayer using nonadditive interaction models. <i>Biophysical Journal</i> , 2009 , 96, 385-402	2.9	52
50	Exploring ion permeation energetics in gramicidin A using polarizable charge equilibration force fields. <i>Journal of the American Chemical Society</i> , 2009 , 131, 13890-1	16.4	51
49	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	3.8	48
48	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, 11641-53	2.4	43
47	Nonadditive empirical force fields for short-chain linear alcohols: methanol to butanol. Hydration free energetics and Kirkwood-Buff analysis using charge equilibration models. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 11076-92	3.4	42
46	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, 9183-96	3.4	40

45	Electrostatic properties of aqueous salt solution interfaces: a comparison of polarizable and nonpolarizable ion models. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 11679-93	3.4	37
44	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	1.9	36
43	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	3.9	35
42	Investigating Hydrophilic Pores in Model Lipid Bilayers Using Molecular Simulations: Correlating Bilayer Properties with Pore-Formation Thermodynamics. <i>Langmuir</i> , 2015 , 31, 6615-31	4	34
41	Revised charge equilibration potential for liquid alkanes. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 8298-310	3.4	34
40	Incorporating Phase-Dependent Polarizability in Non-Additive Electrostatic Models for Molecular Dynamics Simulations of the Aqueous Liquid-Vapor Interface. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 359-373	6.4	33
39	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, 318-29	3.8	30
38	Electrostatic polarization effects and hydrophobic hydration in ethanol-water solutions from molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 767-78	3.4	28
37	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, 2670-82	3.4	26
36	Water Permeation Through DMPC Lipid Bilayers using Polarizable Charge Equilibration Force Fields. <i>Chemical Physics Letters</i> , 2011 , 508, 289-294	2.5	26
35	Molecular dynamics simulations of aqueous ions at the liquid-vapor interface accelerated using graphics processors. <i>Journal of Computational Chemistry</i> , 2011 , 32, 375-85	3.5	26
34	Free energetics of carbon nanotube association in pure and aqueous ionic solutions. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 8154-68	3.4	25
33	Solvation properties of N-acetyl-β-D-glucosamine: molecular dynamics study incorporating electrostatic polarization. <i>Journal of Computational Chemistry</i> , 2011 , 32, 3339-53	3.5	23
32	Improving numerical reproducibility and stability in large-scale numerical simulations on GPUs 2010		23
31	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, 3578-92	3.4	22
30	Temperature dependence and energetics of single ions at the aqueous liquid-vapor interface. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 6512-23	3.4	22
29	Variation of ion polarizability from vacuum to hydration: insights from Hirshfeld partitioning. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 8984-92	2.8	22
28	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, 6716-27	3.6	19

27	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, 9241-54	3.4	19
26	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, 2958-73	3.5	18
25	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	6	18
24	Binding structures of tri-N-acetyl- β -glucosamine in hen egg white lysozyme using molecular dynamics with a polarizable force field. <i>Journal of Computational Chemistry</i> , 2013 , 34, 163-74	3.5	16
23	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, 164-78	3.4	16
22	Solvation Structure and Energetics of Single Ions at the Aqueous Liquid-Vapor Interface. <i>Chemical Physics Letters</i> , 2012 , 527, 22-26	2.5	15
21	Molecular dynamics simulation of hydrated DPPC monolayers using charge equilibration force fields. <i>Journal of Computational Chemistry</i> , 2012 , 33, 141-52	3.5	15
20	Spherical monovalent ions at aqueous liquid-vapor interfaces: interfacial stability and induced interface fluctuations. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 11732-42	3.4	15
19	Dynamics and energetics of hydrophobically confined water. <i>Physical Review E</i> , 2012 , 85, 051506	2.4	15
18	Role of electrostatics in modulating hydrophobic interactions and barriers to hydrophobic assembly. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 8107-17	3.4	14
17	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, 11719-31	3.4	13
16	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, 4490-504	3.4	12
15	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, 11973-92	3.4	12
14	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	3.9	12
13	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, 1892-906	3.6	10
12	. <i>Computing in Science and Engineering</i> , 2013 , 15, 56-65	1.5	10
11	Revised Charge Equilibration Parameters for More Accurate Hydration Free Energies of Alkanes. <i>Chemical Physics Letters</i> , 2010 , 484, 173	2.5	10
10	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, 1453-68	4.2	8

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| 9 | 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, 876-87 | 2.8 | 8 |
| 8 | 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 | 3.5 | 6 |
| 7 | FENZI: GPU-Enabled Molecular Dynamics Simulations of Large Membrane Regions Based on the CHARMM Force Field and PME 2011 , | | 6 |
| 6 | 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 | 3.6 | 5 |
| 5 | Free energetics of carbon nanotube association in aqueous inorganic NaI salt solutions: Temperature effects using all-atom molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1196-212 | 3.5 | 2 |
| 4 | 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, 26779-85 | 3.6 | 2 |
| 3 | Electrostatic contribution from solvent in modulating single-walled carbon nanotube association. <i>Journal of Chemical Physics</i> , 2014 , 141, 114906 | 3.9 | 2 |
| 2 | Pursuing Coordinated Trajectory Progression and Efficient Resource Utilization of GPU-Enabled Molecular Dynamics Simulations. <i>IEEE Design and Test</i> , 2014 , 31, 40-50 | 1.4 | 1 |
| 1 | Modeling Electrostatic Polarization in Biological Solvents 273-308 | | |