Sandeep Patel

List of Publications by Year in Descending Order

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	Insights into Thiol-Aromatic Interactions: A Stereoelectronic Basis for S-H/π Interactions. *Journal of the American Chemical Society*, **2017**, 139, 1842-1855	16.4	54
61	A charge equilibration formalism for treating charge transfer effects in MD simulations: Application to water clusters. *Journal of Computational Chemistry*, **2017**, 38, 1389-1409	3.5	6
60	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	3.6	5
59	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, 6716-27	3.6	19
58	Free energetics of carbon nanotube association in aqueous inorganic NaI salt solutions: Temperature effects using all-atom molecular dynamics simulations. *Journal of Computational Chemistry*, **2015**, 36, 1196-212	3.5	2
57	Protein denaturants at aqueous-hydrophobic interfaces: self-consistent correlation between induced interfacial fluctuations and denaturant stability at the interface. *Journal of Physical Chemistry B*, **2015**, 119, 164-78	3.4	16
56	Investigating Hydrophilic Pores in Model Lipid Bilayers Using Molecular Simulations: Correlating Bilayer Properties with Pore-Formation Thermodynamics. *Langmuir*, **2015**, 31, 6615-31	4	34
55	Association of alkanes with the aqueous liquid-vapor interface: a reference system for interpreting hydrophobicity generally through interfacial fluctuations. *Physical Chemistry Chemical Physics*, **2014**, 16, 26779-85	3.6	2
54	Ion-specific induced fluctuations and free energetics of aqueous protein hydrophobic interfaces: toward connecting to specific-ion behaviors at aqueous liquid-vapor interfaces. *Journal of Physical Chemistry B*, **2014**, 118, 4490-504	3.4	12
53	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, 2670-82	3.4	26
52	Electrostatic contribution from solvent in modulating single-walled carbon nanotube association. *Journal of Chemical Physics*, **2014**, 141, 114906	3.9	2
51	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, 1453-68	4.2	8
50	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, 11973-92	3.4	12
49	Pursuing Coordinated Trajectory Progression and Efficient Resource Utilization of GPU-Enabled Molecular Dynamics Simulations. *IEEE Design and Test*, **2014**, 31, 40-50	1.4	1
48	Liquid-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, 11719-31	3.4	13
47	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, 11641-53	3.4	43
46	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. *Journal of Physical Chemistry B*, **2013**, 117, 3578-92	3.4	22

45	Binding structures of tri-N-acetyl-β-glucosamine in hen egg white lysozyme using molecular dynamics with a polarizable force field. *Journal of Computational Chemistry*, **2013**, 34, 163-74	3.5	16
44	Temperature dependence and energetics of single ions at the aqueous liquid-vapor interface. *Journal of Physical Chemistry B*, **2013**, 117, 6512-23	3.4	22
43	Spherical monovalent ions at aqueous liquid-vapor interfaces: interfacial stability and induced interface fluctuations. *Journal of Physical Chemistry B*, **2013**, 117, 11732-42	3.4	15
42	. *Computing in Science and Engineering*, **2013**, 15, 56-65	1.5	10
41	Solvation Structure and Energetics of Single Ions at the Aqueous Liquid-Vapor Interface. *Chemical Physics Letters*, **2012**, 527, 22-26	2.5	15
40	Molecular dynamics simulation of hydrated DPPC monolayers using charge equilibration force fields. *Journal of Computational Chemistry*, **2012**, 33, 141-52	3.5	15
39	Role of spatial ionic distribution on the energetics of hydrophobic assembly and properties of the water/hydrophobe interface. *Physical Chemistry Chemical Physics*, **2012**, 14, 1892-906	3.6	10
38	Free energetics of carbon nanotube association in pure and aqueous ionic solutions. *Journal of Physical Chemistry B*, **2012**, 116, 8154-68	3.4	25
37	Charge equilibration force fields for molecular dynamics simulations of lipids, bilayers, and integral membrane protein systems. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 318-29	3.8	30
36	Recent applications and developments of charge equilibration force fields for modeling dynamical charges in classical molecular dynamics simulations. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	36
35	Dynamics and energetics of hydrophobically confined water. *Physical Review E*, **2012**, 85, 051506	2.4	15
34	Water Permeation Through DMPC Lipid Bilayers using Polarizable Charge Equilibration Force Fields. *Chemical Physics Letters*, **2011**, 508, 289-294	2.5	26
33	Molecular dynamics simulations of aqueous ions at the liquid-vapor interface accelerated using graphics processors. *Journal of Computational Chemistry*, **2011**, 32, 375-85	3.5	26
32	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, 2958-73	3.5	18
31	Solvation properties of N-acetyl-β-glucosamine: molecular dynamics study incorporating electrostatic polarization. *Journal of Computational Chemistry*, **2011**, 32, 3339-53	3.5	23
30	FENZI: GPU-Enabled Molecular Dynamics Simulations of Large Membrane Regions Based on the CHARMM Force Field and PME **2011**,		6
29	Phase-transfer energetics of small-molecule alcohols across the water-hexane interface: molecular dynamics simulations using charge equilibration models. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 876-87	2.8	8
28	Nonadditive empirical force fields for short-chain linear alcohols: methanol to butanol. Hydration free energetics and Kirkwood-Buff analysis using charge equilibration models. *Journal of Physical Chemistry B*, **2010**, 114, 11076-92	3.4	42

27	Variation of ion polarizability from vacuum to hydration: insights from Hirshfeld partitioning. *Journal of Physical Chemistry A*, **2010**, 114, 8984-92	2.8	22
26	Role of electrostatics in modulating hydrophobic interactions and barriers to hydrophobic assembly. *Journal of Physical Chemistry B*, **2010**, 114, 8107-17	3.4	14
25	Improving numerical reproducibility and stability in large-scale numerical simulations on GPUs **2010** ,		23
24	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	3.9	12
23	Revised Charge Equilibration Parameters for More Accurate Hydration Free Energies of Alkanes. *Chemical Physics Letters*, **2010**, 484, 173	2.5	10
22	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	3.9	35
21	Exploring ion permeation energetics in gramicidin A using polarizable charge equilibration force fields. *Journal of the American Chemical Society*, **2009**, 131, 13890-1	16.4	51
20	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, 9183-96	3.4	40
19	Molecular dynamics simulations of a DMPC bilayer using nonadditive interaction models. *Biophysical Journal*, **2009**, 96, 385-402	2.9	52
18	Incorporating Phase-Dependent Polarizability in Non-Additive Electrostatic Models for Molecular Dynamics Simulations of the Aqueous Liquid-Vapor Interface. *Journal of Chemical Theory and Computation*, **2009**, 5, 359-373	6.4	33
17	Interfacial structure, thermodynamics, and electrostatics of aqueous methanol solutions via molecular dynamics simulations using charge equilibration models. *Journal of Physical Chemistry B*, **2009**, 113, 9241-54	3.4	19
16	Electrostatic polarization effects and hydrophobic hydration in ethanol-water solutions from molecular dynamics simulations. *Journal of Physical Chemistry B*, **2009**, 113, 767-78	3.4	28
15	Electrostatic properties of aqueous salt solution interfaces: a comparison of polarizable and nonpolarizable ion models. *Journal of Physical Chemistry B*, **2008**, 112, 11679-93	3.4	37
14	Origin and control of superlinear polarizability scaling in chemical potential equalization methods. *Journal of Chemical Physics*, **2008**, 128, 144110	3.9	67
13	Comparison of the Solvation Structure of Polarizable and Nonpolarizable Ions in Bulk Water and Near the Aqueous Liquid/Vapor Interface. *Journal of Physical Chemistry C*, **2008**, 112, 7455-7467	3.8	48
12	Revised charge equilibration potential for liquid alkanes. *Journal of Physical Chemistry B*, **2008**, 112, 8298-310	3.4	34
11	Thermodynamic and structural properties of methanol-water solutions using nonadditive interaction models. *Journal of Computational Chemistry*, **2008**, 29, 1142-52	3.5	61
10	Condensed-phase properties of n-alkyl-amines from molecular dynamics simulations using charge equilibration force fields. *Journal of Molecular Liquids*, **2008**, 142, 32-40	6	18

List of Publications

9	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	3.9	97
8	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. *Molecular Simulation*, **2006**, 32, 231-249	2	101
7	Revisiting the hexane-water interface via molecular dynamics simulations using nonadditive alkane-water potentials. *Journal of Chemical Physics*, **2006**, 124, 204706	3.9	54
6	Structure, thermodynamics, and liquid-vapor equilibrium of ethanol from molecular-dynamics simulations using nonadditive interactions. *Journal of Chemical Physics*, **2005**, 123, 164502	3.9	58
5	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	3.9	61
4	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. *Journal of Computational Chemistry*, **2004**, 25, 1-15	3.5	414
3	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, 1504-14	3.5	371
2	Chemical and electrochemical copolymerization of aniline with alkyl ring-substituted anilines. *Macromolecules*, **1990**, 23, 758-764	5.5	235
1	Modeling Electrostatic Polarization in Biological Solvents273-308		