B L Bhargava

List of Publications by Year
in descending order

40 papers	2,216 citations	304743 22 h-index	276875 41 g-index
45 all docs	45 docs citations	45 times ranked	1869 citing authors

#	Article	IF	Citations
1	Refined potential model for atomistic simulations of ionic liquid [bmim][PF6]. Journal of Chemical Physics, 2007, 127, 114510.	3.0	322
2	Nanoscale organization in room temperature ionic liquids: a coarse grained molecular dynamics simulation study. Soft Matter, 2007, 3, 1395.	2.7	194
3	Layering at an Ionic Liquidâ^'Vapor Interface:Â A Molecular Dynamics Simulation Study of [bmim][PF6]. Journal of the American Chemical Society, 2006, 128, 10073-10078.	13.7	177
4	Dynamics in a room-temperature ionic liquid: A computer simulation study of 1,3-dimethylimidazolium chloride. Journal of Chemical Physics, 2005, 123, 144505.	3.0	162
5	Modelling room temperature ionic liquids. Chemical Communications, 2008, , 3339.	4.1	162
6	Intermolecular structure and dynamics in an ionic liquid: A Carâ€"Parrinello molecular dynamics simulation study of 1,3-dimethylimidazolium chloride. Chemical Physics Letters, 2006, 417, 486-491.	2.6	153
7	Insights into the Structure and Dynamics of a Room-Temperature Ionic Liquid:Â Ab Initio Molecular Dynamics Simulation Studies of 1-n-Butyl-3-methylimidazolium Hexafluorophosphate ([bmim][PF6]) and the [bmim][PF6]â^'CO2Mixture. Journal of Physical Chemistry B, 2007, 111, 4477-4487.	2.6	148
8	Probing anionâ€"carbon dioxide interactions in room temperature ionic liquids: Gas phase cluster calculations. Chemical Physics Letters, 2007, 444, 242-246.	2.6	106
9	Computational studies of room temperature ionic liquidâ€"water mixtures. Chemical Communications, 2011, 47, 6228.	4.1	105
10	Molecular Dynamics Studies of Cation Aggregation in the Room Temperature Ionic Liquid [C10mim][Br] in Aqueous Solution. Journal of Physical Chemistry A, 2009, 113, 1898-1904.	2.5	66
11	Aqueous solutions of imidazolium ionic liquids: molecular dynamics studies. Soft Matter, 2009, 5, 3475.	2.7	58
12	Initial Stages of Aggregation in Aqueous Solutions of Ionic Liquids: Molecular Dynamics Studies. Journal of Physical Chemistry B, 2009, 113, 9499-9505.	2.6	51
13	Formation of micelles in aqueous solutions of a room temperature ionic liquid: a study using coarse grained molecular dynamics. Molecular Physics, 2009, 107, 393-401.	1.7	47
14	Formation of Interconnected Aggregates in Aqueous Dicationic Ionic Liquid Solutions. Journal of Chemical Theory and Computation, 2010, 6, 873-879.	5.3	47
15	Molecular dynamics simulation studies of CO₂ â€" [bmim][PF₆] solutions: Effect of CO₂ concentration. AICHE Journal, 2008, 54, 2971-2978.	3.6	46
16	Structural Correlations and Charge Ordering in a Roomâ€Temperature Ionic Liquid. ChemPhysChem, 2008, 9, 67-70.	2.1	45
17	Nanoscale Organization in Aqueous Dicationic Ionic Liquid Solutions. Journal of Physical Chemistry B, 2011, 115, 10439-10446.	2.6	34
18	Ab Initio Molecular Dynamics Simulation of a 1-Ethyl-3-methylimidazolium Fluorideâ^'Hydrogen Fluoride Mixture. Journal of Physical Chemistry B, 2008, 112, 7566-7573.	2.6	30

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19	Surface Structure and Dynamics of Ions at the Liquidâ€“Vapor Interface of Binary Ionic Liquid Mixtures: Molecular Dynamics Studies. Journal of Physical Chemistry C, 2016, 120, 5430-5441.	3.1	30
20	Effect of Cation Asymmetry on the Aggregation in Aqueous 1-Alkyl,3-decylimidazolium Bromide Solutions: Molecular Dynamics Studies. Journal of Physical Chemistry B, 2014, 118, 6241-6249.	2.6	26
21	Ab initio studies on [bmim][PF6]-CO2 mixture and CO2 clusters. Bulletin of Materials Science, 2008, 31, 327-334.	1.7	24
22	Segregation of ions at the interface: molecular dynamics studies of the bulk and liquidâ€“vapor interface structure of equimolar binary mixtures of ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 19919-19928.	2.8	22
23	Hydrogen Evolution from Formic Acid in an Ionic Liquid Solvent: A Mechanistic Study by ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 14136-14140.	2.6	21
24	SixC1â^'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	1.9	16
25	Intermolecular interactions in tetrabutylammonium chloride based deep eutectic solvents: Classical molecular dynamics studies. Journal of Molecular Liquids, 2021, 335, 116139.	4.9	16
26	Nanoclusters of room temperature ionic liquids: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2009, 11, 8745.	2.8	14
27	Effect of spacer chain length on the liquid structure of aqueous dicationic ionic liquid solutions: molecular dynamics studies. Physical Chemistry Chemical Physics, 2015, 17, 11627-11637.	2.8	14
28	Molecular dynamics investigation of non-ionic deep eutectic solvents. Journal of Molecular Graphics and Modelling, 2022, 113, 108152.	2.4	11
29	Glycine molecules in ionic liquid based reverse micelles: Investigation of structure and dynamics using molecular dynamics simulations. Journal of Molecular Liquids, 2017, 230, 384-394.	4.9	10
30	Ionic Liquids at Nonaneâ€“Water Interfaces: Molecular Dynamics Studies. Journal of Physical Chemistry B, 2014, 118, 13930-13939.	2.6	8
31	Self-Assembly of Cations in Aqueous Solutions of Hydroxyl-Functionalized Ionic Liquids: Molecular Dynamics Studies. Journal of Physical Chemistry B, 2015, 119, 11815-11824.	2.6	7
32	Self-Assembly of Cations in Aqueous Solutions of Multiheaded Cationic Surfactants: All Atom Molecular Dynamics Simulation Studies. Journal of Physical Chemistry B, 2018, 122, 10943-10952.	2.6	6
33	Insights into the structure and dynamics at the hexadecane dropletâ€“water interface in the presence of 1-alkanols as emulsifiers: Molecular dynamics studies. Journal of Molecular Liquids, 2017, 234, 249-259.	4.9	4
34	Computational studies of fibrillation induced selective cytotoxicity of cross-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si32.svg"><mml:mrow><mml:mi>Î±</mml:mi></mml:mrow></mml:math> amyloid â€“ Phenol Soluble Modulin <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si33.svg"><mml:mrow><mml:mi>Î±</mml:mi></mml:mrow></mml:math>3. Chemical Physics, 2020, 535, 110777.	1.9	3
35	Solvation of Methyl Lactate in Water: Molecular Dynamics Studies. Journal of Physical Chemistry B, 2018, 122, 2113-2120.	2.6	2
36	Aqueous solutions of hydroxyl-functionalized ionic liquids: Molecular dynamics studies. Journal of Molecular Graphics and Modelling, 2020, 101, 107721.	2.4	2

#	Article	IF	Citations
37	Exploring the candidates for a new protein folding â€“ cross-Î± amyloid â€“ in available protein databases. Physical Chemistry Chemical Physics, 2020, 22, 23725-23734.	2.8	1
38	Helix-coil transition and conformational deformity in AÎ²₄₂-monomer: a case study using the Zn²⁺ cation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8949-8960.	3.5	1
39	The effect of external salts on the aggregation of the multiheaded surfactants: All-atom molecular dynamics studies. Journal of Molecular Graphics and Modelling, 2022, 111, 108110.	2.4	1
40	Molecular dynamics simulations of ionic liquids. , 2021, , 87-104.		0