Sundaram Balasubramanian

List of Publications by Year
in descending order

156 papers	7,989 citations	47 h-index	84 g-index
		47006	54911
164 all docs	164 docs citations	164 times ranked	8009 citing authors

#	Article	IF	Citations
1	Quantitative Sequencing of 5-Methylcytosine and 5-Hydroxymethylcytosine at Single-Base Resolution. Science, 2012, 336, 934-937.	12.6	850
2	Hydrogen-Bond Dynamics near a Micellar Surface: Origin of the Universal Slow Relaxation at Complex Aqueous Interfaces. Physical Review Letters, 2002, 89, 115505.	7.8	345
3	Refined potential model for atomistic simulations of ionic liquid [bmim][PF6]. Journal of Chemical Physics, 2007, 127, 114510.	3.0	322
4	Are There Stable Ion-Pairs in Room-Temperature Ionic Liquids? Molecular Dynamics Simulations of 1-n-Butyl-3-methylimidazolium Hexafluorophosphate. Journal of the American Chemical Society, 2009, 131, 15825-15833.	13.7	283
5	Nanoscale organization in room temperature ionic liquids: a coarse grained molecular dynamics simulation study. Soft Matter, 2007, 3, 1395.	2.7	194
6	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
7	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
8	Modelling room temperature ionic liquids. Chemical Communications, 2008, , 3339.	4.1	162
9	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
10	Self-Sorted, Random, and Block Supramolecular Copolymers via Sequence Controlled, Multicomponent Self-Assembly. Journal of the American Chemical Society, 2020, 142, 7606-7617.	13.7	151
11	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
12	Biomimetic temporal self-assembly via fuel-driven controlled supramolecular polymerization. Nature Communications, 2018, 9, 1295.	12.8	148
13	What Molecular Features Govern the Mechanism of Supramolecular Polymerization?. ChemPhysChem, 2013, 14, 661-673.	2.1	134
14	Modified nonequilibrium molecular dynamics for fluid flows with energy conservation. Journal of Chemical Physics, 1997, 106, 5615-5621.	3.0	130
15	Amide Functionalized Microporous Organic Polymer (Am-MOP) for Selective CO₂ Sorption and Catalysis. ACS Applied Materials & Interfaces, 2014, 6, 4630-4637.	8.0	124
16	Dipole-Moment-Driven Cooperative Supramolecular Polymerization. Journal of the American Chemical Society, 2015, 137, 3924-3932.	13.7	115
17	Flexible and Rigid Amineâ€Functionalized Microporous Frameworks Based on Different Secondary Building Units: Supramolecular Isomerism, Selective CO₂ Capture, and Catalysis. Chemistry - A European Journal, 2014, 20, 4347-4356.	3.3	113
18	Probing anionâ€“carbon dioxide interactions in room temperature ionic liquids: Gas phase cluster calculations. Chemical Physics Letters, 2007, 444, 242-246.	2.6	106

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19	Quantitative Prediction of Physical Properties of Imidazolium Based Room Temperature Ionic Liquids through Determination of Condensed Phase Site Charges: A Refined Force Field. Journal of Physical Chemistry B, 2014, 118, 3409-3422.	2.6	106
20	Identity, Energy, and Environment of Interfacial Water Molecules in a Micellar Solution. Journal of Physical Chemistry B, 2003, 107, 5194-5202.	2.6	99
21	The effects of pressure on structural and dynamical properties of associated liquids: Molecular dynamics calculations for the extended simple point charge model of water. Journal of Chemical Physics, 1997, 107, 8561-8567.	3.0	95
22	Sensitivity of Polar Solvation Dynamics to the Secondary Structures of Aqueous Proteins and the Role of Surface Exposure of the Probe. Journal of the American Chemical Society, 2005, 127, 4071-4075.	13.7	92
23	A molecular dynamics study of the mixed alkali effect in silicate glasses. Journal of Non-Crystalline Solids, 1995, 181, 157-174.	3.1	90
24	Electron Donorâ^'Acceptor Interactions in Ethanolâ^'CO2Mixtures:Â An Ab Initio Molecular Dynamics Study of Supercritical Carbon Dioxideâ€. Journal of Physical Chemistry B, 2006, 110, 3782-3790.	2.6	88
25	Hydration Layer of a Cationic Micelle, C10TAB:â€‰ Structure, Rigidity, Slow Reorientation, Hydrogen Bond Lifetime, and Solvation Dynamics. Journal of Physical Chemistry B, 2005, 109, 12879-12890.	2.6	86
26	Dynamics of bound and free water in an aqueous micellar solution: Analysis of the lifetime and vibrational frequencies of hydrogen bonds at a complex interface. Physical Review E, 2003, 67, 061502.	2.1	83
27	Correlation between Dynamic Heterogeneity and Local Structure in a Roomâ€Temperature Ionic Liquid: A Molecular Dynamics Study of [bmim][PF‹sub›6‹/sub›]. ChemPhysChem, 2010, 11, 2001-2010.	2.1	82
28	Unusual room temperature CO2 uptake in a fluoro-functionalized MOF: insight from Raman spectroscopy and theoretical studies. Chemical Communications, 2012, 48, 8487.	4.1	78
29	Slow Orientational Dynamics of Water Molecules at a Micellar Surface. Journal of Physical Chemistry B, 2002, 106, 3668-3672.	2.6	77
30	Slow Solvation Dynamics near an Aqueous Micellar Surface. Journal of Physical Chemistry B, 2001, 105, 12529-12533.	2.6	76
31	Shear viscosity of polar fluids: Molecular dynamics calculations of water. Journal of Chemical Physics, 1996, 105, 11190-11195.	3.0	75
32	Density Functional Theory Investigations on the Structure and Dissolution Mechanisms for Cellobiose and Xylan in an Ionic Liquid: Gas Phase and Cluster Calculations. Journal of Physical Chemistry B, 2012, 116, 833-840.	2.6	74
33	Monte Carlo investigations of hexadecane films on a metal substrate. Journal of Chemical Physics, 1995, 103, 3184-3195.	3.0	69
34	Temperature dependence of water dynamics at an aqueous micellar surface: Atomistic molecular dynamics simulation studies of a complex system. Journal of Chemical Physics, 2002, 117, 2852-2859.	3.0	69
35	Ab initio molecular-dynamics study of supercritical carbon dioxide. Journal of Chemical Physics, 2004, 120, 9694-9702.	3.0	67
36	The surface structure of ionic liquids: Comparing simulations with x-ray measurements. Journal of Chemical Physics, 2006, 125, 174715.	3.0	67

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37	Preferential paths in alkali ion migration and the mixed alkali effect in silicate glasses. The Journal of Physical Chemistry, 1993, 97, 8835-8838.	2.9	66
38	Three-Dimensional Metalâ€“Organic Framework with Highly Polar Pore Surface: H₂ and CO₂ Storage Characteristics. Inorganic Chemistry, 2012, 51, 7103-7111.	4.0	66
39	Studying long-time dynamics of imidazolium-based ionic liquids with a systematically coarse-grained model. Physical Chemistry Chemical Physics, 2010, 12, 4714.	2.8	65
40	Evolution of Intermolecular Structure and Dynamics in Supercritical Carbon Dioxide with Pressure:Â An ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2007, 111, 387-392.	2.6	61
41	Supramolecular Polymerization of Benzene-1,3,5-tricarboxamide: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 5218-5228.	2.6	61
42	Autoresolution of Segregated and Mixed pâ€n Stacks by Stereoselective Supramolecular Polymerization in Solution. Angewandte Chemie - International Edition, 2015, 54, 13053-13057.	13.8	61
43	Separation/purification of ethylene from an acetylene/ethylene mixture in a pillared-layer porous metalâ€“organic framework. Chemical Communications, 2017, 53, 4907-4910.	4.1	61
44	Atomistic Simulation Study of the Coupled Motion of Amino Acid Residues and Water Molecules around Protein HP-36: Fluctuations at and around the Active Sites. Journal of Physical Chemistry B, 2004, 108, 12608-12616.	2.6	60
45	Equilibrium and non-equilibrium simulation studies of fluid alkanes in bulk and at interfaces. Faraday Discussions, 1996, 104, 17.	3.2	57
46	Synthesis, Characterization, and Modeling of a Functional Conjugated Microporous Polymer: CO₂ Storage and Light Harvesting. Journal of Physical Chemistry C, 2014, 118, 24369-24376.	3.1	53
47	Molecular dynamics simulations of ionic liquidâ€“vapour interfaces: effect of cation symmetry on structure at the interface. Physical Chemistry Chemical Physics, 2011, 13, 2714-2722.	2.8	48
48	Dynamic Entangled Porous Framework for Hydrocarbon (C2â€“C3) Storage, CO₂ Capture, and Separation. Chemistry - A European Journal, 2016, 22, 6059-6070.	3.3	48
49	Measuring single-molecule nucleic acid dynamics in solution by two-color filtered ratiometric fluorescence correlation spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 14425-14430.	7.1	47
50	Dissolution of cellulose in ionic liquids: an ab initio molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2014, 16, 17458-17465.	2.8	47
51	Understanding SO₂ Capture by Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 4457-4466.	2.6	47
52	Molecular dynamics simulation studies of CO₂ â€“ [bmim][PF₆] solutions: Effect of CO₂ concentration. AICHE Journal, 2008, 54, 2971-2978.	3.6	46
53	Crystal Dynamics in Multiâ€stimuliâ€Responsive Entangled Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2016, 22, 15864-15873.	3.3	46
54	Structural Correlations and Charge Ordering in a Roomâ€Temperature Ionic Liquid. ChemPhysChem, 2008, 9, 67-70.	2.1	45

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55	Shear Viscosity of the Ionic Liquid 1-n-Butyl 3-Methylimidazolium Hexafluorophosphate [bmim][PF₆] Computed by Reverse Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry B, 2008, 112, 8129-8133.	2.6	45
56	Low Frequency Vibrational Modes of Room Temperature Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 1874-1880.	2.6	44
57	Charge-transfer complexation between naphthalene diimides and aromatic solvents. Physical Chemistry Chemical Physics, 2014, 16, 14661.	2.8	44
58	Dissolution of Cellulose in Room Temperature Ionic Liquids: Anion Dependence. Journal of Physical Chemistry B, 2015, 119, 1654-1659.	2.6	44
59	Aqueous Solution of [bmim][PF₆]: Ion and Solvent Effects on Structure and Dynamics. Journal of Physical Chemistry B, 2009, 113, 4799-4806.	2.6	41
60	Homogenous mixing of ionic liquids: molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 21077.	2.8	41
61	Cooperativity in the stacking of benzene-1,3,5-tricarboxamide: The role of dispersion. Chemical Physics Letters, 2011, 515, 226-230.	2.6	39
62	A Refined All-Atom Potential for Imidazolium-Based Room Temperature Ionic Liquids: Acetate, Dicyanamide, and Thiocyanate Anions. Journal of Physical Chemistry B, 2015, 119, 11041-11051.	2.6	39
63	Supramolecular Polymerization: A Coarse Grained Molecular Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 5738-5746.	2.6	38
64	Recent advances in modeling green solvents. Current Opinion in Green and Sustainable Chemistry, 2017, 5, 37-43.	5.9	38
65	Atomistic simulations of ammonium-based protic ionic liquids: steric effects on structure, low frequency vibrational modes and electrical conductivity. Physical Chemistry Chemical Physics, 2015, 17, 4625-4633.	2.8	36
66	Orientational Ordering of Ionic Liquids near a Charged Mica Surface. ChemPhysChem, 2012, 13, 1764-1771.	2.1	35
67	A Molecular Dynamics Study of Collective Transport Properties of Imidazolium-Based Room-Temperature Ionic Liquids. Journal of Chemical & Engineering Data, 2014, 59, 3061-3068.	1.9	34
68	Role of Cation Symmetry in Intermolecular Structure and Dynamics of Room Temperature Ionic Liquids: Simulation Studies. Journal of Physical Chemistry B, 2010, 114, 6455-6463.	2.6	33
69	Simulation Studies of Ultrathin Films of Linear and Branched Alkanes on a Metal Substrate. The Journal of Physical Chemistry, 1996, 100, 11960-11963.	2.9	32
70	Enhanced Molecular Multipole Moments and Solvent Structure in Supercritical Carbon Dioxide. ChemPhysChem, 2004, 5, 1442-1445.	2.1	31
71	Low-Symmetry Self-Assembled Coordination Complexes with Exclusive Diastereoselectivity: Experimental and Computational Studies. Inorganic Chemistry, 2020, 59, 12884-12894.	4.0	31
72	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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73	Hostâ€“Guest [2+2] Cycloaddition Reaction: Postsynthetic Modulation of CO₂ Selectivity and Magnetic Properties in a Bimodal Metalâ€“Organic Framework. Chemistry - A European Journal, 2016, 22, 7792-7799.	3.3	30
74	Tailoring a robust Al-MOF for trapping C₂H₆ and C₂H₂ towards efficient C₂H₄ purification from quaternary mixtures. Chemical Science, 2022, 13, 7172-7180.	7.4	30
75	Ab initio molecular dynamics study of supercritical carbon dioxide including dispersion corrections. Journal of Chemical Physics, 2009, 131, 144506.	3.0	29
76	Carbonic acid: molecule, crystal and aqueous solution. Chemical Communications, 2014, 50, 503-514.	4.1	29
77	Anomalous dielectric relaxation of water molecules at the surface of an aqueous micelle. Journal of Chemical Physics, 2004, 120, 1912-1920.	3.0	28
78	Liquid Dimethyl Carbonate: A Quantum Chemical and Molecular Dynamics Study. Journal of Physical Chemistry B, 2012, 116, 14892-14902.	2.6	28
79	Effect of Pillar Modules and Their Stoichiometry in 3D Porous Frameworks of Zn(II) with [Fe(CN)₆]^{3â€“}: High CO₂/N₂ and CO₂/CH₄ Selectivity. Inorganic Chemistry, 2013, 52, 11385-11397.	4.0	25
80	Ab initio studies on [bmim][PF6]-CO2 mixture and CO2 clusters. Bulletin of Materials Science, 2008, 31, 327-334.	1.7	24
81	Profile unbiased thermostat with dynamical streaming velocities. Journal of Chemical Physics, 1996, 105, 11183-11189.	3.0	23
82	n-Heptane under Pressure:Â Structure and Dynamics from Molecular Simulations. Journal of Physical Chemistry B, 2005, 109, 1936-1946.	2.6	22
83	External electric field reverses helical handedness of a supramolecular columnar stack. Chemical Communications, 2015, 51, 16049-16052.	4.1	22
84	Two 3D metalâ€“organic frameworks of Cd(<scp>ii</scp>): modulation of structures and porous properties based on linker functionalities. CrystEngComm, 2014, 16, 4877-4885.	2.6	21
85	Bioinspired, ATP-driven co-operative supramolecular polymerization and its pathway dependence. Chemical Communications, 2020, 56, 1505-1508.	4.1	21
86	Vibrational Signatures of Cationâ€“Anion Hydrogen Bonding in Ionic Liquids: A Periodic Density Functional Theory and Molecular Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 1994-2002.	2.6	20
87	Nonequilibrium Molecular Dynamics. Reviews in Computational Chemistry, 2007, , 291-397.	1.5	19
88	Effect of cation symmetry on the organization of ionic liquids near a charged mica surface. Journal of Physics Condensed Matter, 2014, 26, 284101.	1.8	19
89	Fluorocarbon-Functionalized Superhydrophobic Metalâ€“Organic Framework: Enhanced CO₂ Uptake via Photoinduced Postsynthetic Modification. Inorganic Chemistry, 2021, 60, 3823-3833.	4.0	19
90	Emergence of nanoscale order in room temperature ionic liquids: simulation of symmetric 1,3-didecylimidazolium hexafluorophosphate. Journal of Materials Chemistry, 2009, 19, 4343.	6.7	18

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91	A molecular dynamics study of amorphous selenium. Chemical Physics, 1992, 166, 131-137.	1.9	16
92	Hydrodynamic boundary conditions for confined fluids via a nonequilibrium molecular dynamics simulation. Journal of Chemical Physics, 1996, 105, 3211-3214.	3.0	16
93	An atomistic simulation study of a solid monolayer and trilayer ofn-hexane on graphite. Journal of Chemical Physics, 2003, 118, 5082-5086.	3.0	16
94	Computational and Experimental Studies of Molecularly Imprinted Polymers for Organochlorine Pesticides Heptachlor and DDT. Current Analytical Chemistry, 2012, 8, 562-568.	1.2	16
95	Molecular Mechanism behind Solvent Concentration-Dependent Optimal Activity of Thermomyces lanuginosus Lipase in a Biocompatible Ionic Liquid: Interfacial Activation through Arginine Switch. Journal of Physical Chemistry B, 2016, 120, 11720-11732.	2.6	16
96	Structureâ€“Property Relationships in Amorphous Microporous Polymers. Journal of Physical Chemistry B, 2016, 120, 557-565.	2.6	16
97	Molecular Dynamics Investigation of Structure and Transport in the K2O-2SiO2 System Using a Partial Charge Based Model Potential. The Journal of Physical Chemistry, 1994, 98, 10871-10880.	2.9	15
98	Differentiating the mechanism of self-assembly in supramolecular polymers through computation. Chemical Communications, 2019, 55, 3773-3776.	4.1	15
99	A Molecular Dynamics Study of Atomic Correlations in Glassy B2S3. The Journal of Physical Chemistry, 1994, 98, 9216-9221.	2.9	14
100	Vibrational dynamics of solid poly(ethylene oxide). Physical Review B, 2003, 68, .	3.2	14
101	Nanoclusters of room temperature ionic liquids: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2009, 11, 8745.	2.8	14
102	Vibrational Spectra of Linear Oligomers of Carbonic Acid: A Quantum Chemical Study. Journal of Physical Chemistry A, 2012, 116, 1638-1647.	2.5	14
103	Phase behaviour of ultrathin crystalline n-heptane films on graphite: An atomistic simulation study. Physical Chemistry Chemical Physics, 2005, 7, 2044.	2.8	13
104	Ab initio molecular dynamics investigations of structural, electronic and dynamical properties of water in supercritical carbon dioxide. Indian Journal of Physics, 2009, 83, 13-29.	1.8	13
105	Theoretical investigations of candidate crystal structures for Î²-carbonic acid. Journal of Chemical Physics, 2011, 134, 124511.	3.0	13
106	Editorial: Ionic Liquids: The Fundamentals and Forces Driving Their Rise. ChemPhysChem, 2012, 13, 1603-1603.	2.1	13
107	Charge Environment and Hydrogen Bond Dynamics in Binary Ionic Liquid Mixtures: A Computational Study. Journal of Physical Chemistry Letters, 2018, 9, 3511-3516.	4.6	13
108	Orientational Switch of the Lipase A Enzyme at the Oilâ€“Water Interface: An Order of Magnitude Increase in Turnover Rate with a Single Surfactant Tag Explained. Journal of Physical Chemistry Letters, 2020, 11, 2977-2982.	4.6	13

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109	Trimethylaluminum:Â A Computer Study of the Condensed Phases and the Gas Dimer. Journal of Physical Chemistry B, 1998, 102, 10136-10141.	2.6	12
110	Response to â€œComment on â€˜Modified nonequilibrium molecular dynamics for fluid flows with energy conservationâ€™â€‰â€•[J. Chem. Phys. 108, 4351 (1998)]. Journal of Chemical Physics, 1998, 108, 4353-4354.	3.0	12
111	Molecular modelling of supramolecular one dimensional polymers. RSC Advances, 2018, 8, 22659-22669.	3.6	12
112	Refined Force Field for Liquid Sulfolane with Particular Emphasis to Its Transport Characteristics. ACS Omega, 2020, 5, 28285-28295.	3.5	12
113	Hopping in High Concentration Electrolytes - Long Time Bulk and Single-Particle Signatures, Free Energy Barriers, and Structural Insights. Journal of Physical Chemistry Letters, 2020, 11, 9613-9620.	4.6	12
114	Computer simulation study of water using a fluctuating charge model. Journal of Chemical Sciences, 2001, 113, 579-590.	1.5	11
115	Proton Hopping Mechanisms in a Protic Organic Ionic Plastic Crystal. Journal of Physical Chemistry C, 2016, 120, 22903-22909.	3.1	11
116	Thermal phase behavior and ion hopping in a 1,2,4-triazolium perfluorobutanesulfonate protic organic ionic plastic crystal. Physical Chemistry Chemical Physics, 2016, 18, 2047-2053.	2.8	11
117	Understanding the self-assembly of amino ester-based benzene-1,3,5-tricarboxamides using molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 258-266.	2.8	11
118	Efficient Parametrization of Force Field for the Quantitative Prediction of the Physical Properties of Ionic Liquid Electrolytes. Journal of Chemical Theory and Computation, 2021, 17, 4274-4290.	5.3	11
119	A Dynamic Chemical Clip in Supramolecular Framework for Sorting Alkylaromatic Isomers using Thermodynamic and Kinetic Preferences. Angewandte Chemie - International Edition, 2021, 60, 19921-19927.	13.8	11
120	Two for one: propylene carbonate co-solvent for high performance aqueous zinc-ion batteries â€“ remedies for persistent issues at both electrodes. Journal of Materials Chemistry A, 2022, 10, 12597-12607.	10.3	11
121	Slow ligand-induced conformational switch increases the catalytic rate in Plasmodium falciparum hypoxanthine guanine xanthine phosphoribosyltransferase. Molecular BioSystems, 2015, 11, 1410-1424.	2.9	10
122	Supramolecular Polymerization of N,Nâ€²,Nâ€³,Nâ€´-tetra-(Tetradecyl)-1,3,6,8-pyrenetetracarboxamide: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 11492-11503.	2.6	10
123	Computation of the hydrodynamic boundary parameters of a confined fluid via non-equilibrium molecular dynamics. Physica A: Statistical Mechanics and Its Applications, 1997, 240, 305-314.	2.6	9
124	CO₂ Migration Pathways in Oxalate Decarboxylase and Clues about Its Active Site. Journal of Physical Chemistry B, 2013, 117, 12451-12460.	2.6	9
125	Electronegativities of constituent atoms and Tc of superconductors. Solid State Communications, 1989, 71, 979-982.	1.9	8
126	Structure of solid monolayers and multilayers ofn-hexane on graphite. Journal of Chemical Sciences, 2003, 115, 663-677.	1.5	8

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127	Orderâ€“disorder transitions and melting in a helical polymer crystal: molecular dynamics calculations of model poly(ethylene oxide). Chemical Physics Letters, 2004, 385, 351-356.	2.6	8
128	pH-Induced Rotation of Lidless Lipase LipA from Bacillus subtilis at Lipaseâ€“Detergent Interface. Journal of Physical Chemistry B, 2018, 122, 4802-4812.	2.6	8
129	An atomistic view of solvent-free protein liquids: the case of Lipase A. Physical Chemistry Chemical Physics, 2021, 23, 7302-7312.	2.8	8
130	A Molecular Dynamics Investigation of the Structures and Mixed Alkali Effect in Sulfate Glasses. Journal of Solid State Chemistry, 1993, 106, 174-183.	2.9	7
131	Modelling Gas Adsorption in Porous Solids: Roles of Surface Chemistry and Pore Architecture. Journal of Chemical Sciences, 2015, 127, 1687-1699.	1.5	7
132	Molecular Dynamics Investigation of Efficient SO2 Absorption by Anion-Functionalized Ionic Liquids. Journal of Chemical Sciences, 2017, 129, 859-872.	1.5	7
133	Calculation of friction coefficient of a solid-liquid interface via a non-equilibrium molecular dynamics simulation. Bulletin of Materials Science, 1999, 22, 873-876.	1.7	6
134	Insights into the Stabilization of Fluoride Ions in Ionic Liquids: Pointers to Better Fluorinating Agents. Journal of Physical Chemistry B, 2020, 124, 8844-8856.	2.6	6
135	Structural basis for the hyperthermostability of an archaeal enzyme induced by succinimide formation. Biophysical Journal, 2021, 120, 3732-3746.	0.5	5
136	Thermally activated dynamic gating underlies higher gas adsorption at higher temperatures in metalâ€“organic frameworks. Journal of Materials Chemistry A, 2021, 9, 27398-27407.	10.3	5
137	Dynamic Atomic Force Microscopy for Ionic Liquids: Massless Model Shows the Way. ChemPhysChem, 2012, 13, 3085-3086.	2.1	4
138	Product Release Pathways in Human and Plasmodium falciparum Phosphoribosyltransferase. Journal of Chemical Information and Modeling, 2016, 56, 1528-1538.	5.4	4
139	Liquid ethylene glycol: prediction of physical properties, conformer population and interfacial enrichment with a refined non-polarizable force field. Physical Chemistry Chemical Physics, 2022, 24, 10985-10992.	2.8	4
140	Enhanced Molecular Multipole Moments and Solvent Structure in Supercritical Carbon Dioxide. ChemPhysChem, 2006, 7, 1167-1167.	2.1	3
141	Intermolecular correlations in an ionic liquid under shear. Journal of Physics Condensed Matter, 2009, 21, 035105.	1.8	3
142	Elucidating the interaction of H 2 O 2 with polar amino acids â€“ Quantum chemical calculations. Chemical Physics Letters, 2014, 613, 5-9.	2.6	3
143	Structural and dynamical correlations in PfHGXPRT oligomers: A molecular dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1590-1605.	3.5	3
144	Insights into substrate behavior in a solvent-free protein liquid to rationalize its reduced catalytic rate. RSC Advances, 2022, 12, 11896-11905.	3.6	3

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145	Superconductivity in TmBa2Cu3O9-x. Journal of Physics C: Solid State Physics, 1987, 20, L621-L626.	1.5	2
146	Argon multilayers on a corrugated surface: effect of coverage on structure. Chemical Physics Letters, 2002, 362, 144-150.	2.6	2
147	Role of W181 in modulating kinetic properties of Plasmodium falciparum hypoxanthine guanine xanthine phosphoribosyltransferase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1658-1669.	2.6	2
148	Molecular Dynamics and Free Energy Simulations of Phenylacetate and CO₂ Release from AMDase and Its G74C/C188S Mutant: A Possible Rationale for the Reduced Activity of the Latter. Journal of Physical Chemistry B, 2016, 120, 11644-11653.	2.6	2
149	Dipolar relaxation in thin films of supramolecular stacks of benzenecarboxamides and insights to enhance their ferroelectric characteristics. Physical Chemistry Chemical Physics, 2021, 23, 3152-3159.	2.8	2
150	Gate Opening without Volume Change Triggers Cooperative Gas Interactions, Underpins an Isotherm Step in Metalâ€“Organic Frameworks. Inorganic Chemistry, 2022, 61, 10810-10821.	4.0	2
151	Modelling adsorption in fluorinated TKL MOFs. Molecular Simulation, 2017, 43, 213-221.	2.0	1
152	Unraveling the Sorption Mechanism of CO₂ in a Molecular Crystal without Intrinsic Porosity. Journal of Physical Chemistry B, 2019, 123, 7471-7481.	2.6	1
153	Dynamics of water at surface of complex systems: Study of aqueous micelles and proteins. , 2004, , 213-220.		0
154	How a purine salvage enzyme singles out the right base. Journal of Biological Chemistry, 2019, 294, 11992-11993.	3.4	0
155	A Dynamic Chemical Clip in Supramolecular Framework for Sorting Alkylaromatic Isomers using Thermodynamic and Kinetic Preferences. Angewandte Chemie, 2021, 133, 20074-20080.	2.0	0
156	Computational Modelling of Charge Transport through Molecular Devices. , 2019, , 429-452.		0