Jayendran C Rasaiah

List of Publications by Year
in descending order

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61 papers	5,312 citations	147566 31 h-index	123241 61 g-index
73 all docs	73 docs citations	73 times ranked	4062 citing authors

#	Article	IF	Citations
1	Exchange Functionals and Basis Sets for Density Functional Theory Studies of Water Splitting on Selected ZnO Nanocluster Catalysts. ACS Omega, 2022, 7, 12556-12569.	1.6	7
2	Water-Mediated Interactions Determine Helix Formation of Peptides in Open Nanotubes. Journal of Physical Chemistry B, 2021, 125, 817-824.	1.2	1
3	Lightâ€“Nucleotide versus Ionâ€“Nucleotide Interactions for Single-Nucleotide Resolution. Journal of Physical Chemistry B, 2021, 125, 2863-2870.	1.2	0
4	Theoretical study of the stability, structure, and optical spectra of small silver clusters and their formation using density functional theory. Physical Chemistry Chemical Physics, 2021, 23, 25507-25517.	1.3	8
5	Reverse Translocation of Nucleotides through a Carbon Nanotube. Journal of Physical Chemistry B, 2020, 124, 937-943.	1.2	2
6	Molecular Dynamics Simulation Study of Transverse and Longitudinal Ionic Currents in Solid-State Nanopore DNA Sequencing. ACS Applied Nano Materials, 2020, 3, 1438-1447.	2.4	13
7	Nanocluster Growth and Coalescence Modulated by Ligands. Journal of Physical Chemistry C, 2020, 124, 17340-17346.	1.5	3
8	Acetic acid and propionic acid decarboxylation on Mg(OH)2 nanoclusters: a density functional theory study. Journal of Materials Science, 2020, 55, 16914-16927.	1.7	0
9	Ligand-Mediated Nanocluster Formation with Classical and Autocatalytic Growth. Journal of Physical Chemistry C, 2019, 123, 29954-29963.	1.5	6
10	Thermodynamics of Helixâ€“Coil Transitions of Polyalanine in Open Carbon Nanotubes. Journal of Physical Chemistry Letters, 2017, 8, 494-499.	2.1	3
11	Proton transfer and the diffusion of H+ and OHâ^' ions along water wires. Journal of Chemical Physics, 2013, 139, 124507.	1.2	30
12	Entropy of single-file water in (6,6) carbon nanotubes. Journal of Chemical Physics, 2012, 137, 044709.	1.2	43
13	Proton transfer and the mobilities of the H+ and OHâ^' ions from studies of a dissociating model for water. Journal of Chemical Physics, 2011, 135, 124505.	1.2	170
14	Water in the Polar and Nonpolar Cavities of the Protein Interleukin-1Î². Journal of Physical Chemistry B, 2010, 114, 16290-16297.	1.2	39
15	Proton transfer reactions of halogenated compounds: Using gas chromatography/Fourier transform ion cyclotron resonance mass spectrometry (GC/FT-ICR MS) and ab initio calculations. International Journal of Mass Spectrometry, 2010, 293, 1-11.	0.7	7
16	Local dynamics and structure of the solvated hydroxide ion in water. Molecular Simulation, 2010, 36, 69-73.	0.9	10
17	Reaction coordinates for electron transfer reactions. Journal of Chemical Physics, 2008, 129, 214503.	1.2	7
18	Water in Nonpolar Confinement: From Nanotubes to Proteins and Beyond. Annual Review of Physical Chemistry, 2008, 59, 713-740.	4.8	624

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19	Metastable Water Clusters in the Nonpolar Cavities of the Thermostable Protein Tetrabrachion. Journal of the American Chemical Society, 2007, 129, 7369-7377.	6.6	75
20	Structural and Dynamic Properties of Concentrated Alkali Halide Solutions:Â A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 209-217.	1.2	117
21	Water between Plates in the Presence of an Electric Field in an Open Systemâ€. Journal of Physical Chemistry B, 2005, 109, 6629-6635.	1.2	85
22	Water clusters in nonpolar cavities. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 17002-17005.	3.3	222
23	Electric field and temperature effects on water in the narrow nonpolar pores of carbon nanotubes. Journal of Chemical Physics, 2004, 121, 7955.	1.2	197
24	Filling and emptying kinetics of carbon nanotubes in water. Journal of Chemical Physics, 2002, 117, 10789-10795.	1.2	224
25	Computer simulation studies of the structure and dynamics of ions and nonâ€“polar solutes in water. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2001, 359, 1545-1574.	1.6	77
26	Computer simulation studies of aqueous solutions at ambient and supercritical conditions using effective pair potential and polarizable potential models for water. Journal of Chemical Physics, 2001, 114, 7544-7555.	1.2	85
27	Computer simulation studies of aqueous sodium chloride solutions at 298 K and 683 K. Journal of Chemical Physics, 2000, 113, 8125-8137.	1.2	148
28	Structure of Aqueous Solutions of Ions and Neutral Solutes at Infinite Dilution at a Supercritical Temperature of 683 K. Journal of the American Chemical Society, 2000, 122, 11182-11193.	6.6	54
29	Dynamics of Aqueous Solutions of Ions and Neutral Solutes at Infinite Dilution at a Supercritical Temperature of 683 K. Journal of the American Chemical Society, 2000, 122, 11194-11202.	6.6	58
30	Solvent Structure, Dynamics, and Ion Mobility in Aqueous Solutions at 25 Â°C. Journal of Physical Chemistry B, 1998, 102, 4193-4204.	1.2	857
31	Friction Coefficients of Ions in Aqueous Solution at 25 Â°C. Journal of the American Chemical Society, 1998, 120, 12041-12050.	6.6	78
32	Phase transitions of quadrupolar fluids. Journal of Chemical Physics, 1997, 107, 237-242.	1.2	14
33	Molecular Dynamics Simulation of Ion Mobility. 2. Alkali Metal and Halide Ions Using the SPC/E Model for Water at 25 Â°Câ€. The Journal of Physical Chemistry, 1996, 100, 1420-1425.	2.9	464
34	Mobility and solvation of ions in channels. Journal of Chemical Physics, 1996, 105, 9266-9280.	1.2	205
35	Solvent dynamics and electron transfer reactions. AIP Conference Proceedings, 1994, , .	0.3	2
36	Molecular dynamics simulation of ionic mobility. I. Alkali metal cations in water at 25â€‰Â°C. Journal of Chemical Physics, 1994, 101, 6964-6974.	1.2	199

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37	Solvent dynamical effects on electron transfer reactions. Journal of Chemical Physics, 1994, 101, 9966-9981.	1.2	21
38	An integral equation approximation for the dynamics of reversible electronâ€transfer reactions. Journal of Chemical Physics, 1993, 98, 1213-1227.	1.2	24
39	Reversible electron transfer dynamics in nonâ€Debye solvents. Journal of Chemical Physics, 1992, 96, 1435-1443.	1.2	28
40	Dynamics of reversible electron transfer reactions. Journal of Chemical Physics, 1991, 95, 3325-3340.	1.2	42
41	Unsymmetrical electrolytes with adhesive interactions. Journal of Chemical Physics, 1991, 94, 3141-3149.	1.2	18
42	Cavity functions and association in models for weak electrolytes and sticky hard spheres. Journal of Chemical Physics, 1990, 92, 7554-7564.	1.2	19
43	Fluctuation dominated recombination kinetics with traps. Journal of Chemical Physics, 1990, 93, 5768-5774.	1.2	19
44	Solvent effects in weak electrolytes. II. Dipolar hard sphere solvent and the sticky electrolyte model with L=Ïƒ. Journal of Chemical Physics, 1989, 91, 505-516.	1.2	10
45	Solvent effects in weak electrolytes. I. Effect of a hard sphere solvent on the sticky electrolyte model with L=Ïƒ. Journal of Chemical Physics, 1989, 91, 495-504.	1.2	9
46	Molecular dynamics study of a dipolar fluid between charged plates. II. Journal of Chemical Physics, 1987, 86, 2383-2393.	1.2	36
47	Chemical ion association and dipolar dumbbells in the mean spherical approximation. Journal of Chemical Physics, 1987, 86, 983-994.	1.2	29
48	Molecular dynamics study of a dipolar fluid between charged plates. Journal of Chemical Physics, 1986, 85, 5232-5237.	1.2	38
49	The equilibrium properties of charged hard spheres with adhesive interactions between oppositely charged ions. Journal of Chemical Physics, 1985, 83, 6396-6404.	1.2	29
50	Ion association and dipolar dumbbells: Solutions of the HNC and HNC/MS approximations atL=Ïƒ/2 and Ïƒ/3 for the sticky electrolyte model. Journal of Chemical Physics, 1985, 83, 5870-5881.	1.2	34
51	A model for association in electrolytes. Analytic solution of the hypernettedâ€chain/mean spherical approximation. Journal of Chemical Physics, 1985, 83, 317-325.	1.2	58
52	Electrostriction and the dielectric constant of a simple polar fluid. Journal of Chemical Physics, 1982, 77, 5710-5713.	1.2	14
53	Polarization density profiles for dipoles against an electrified wall in the MS and RLHNC approximations. Journal of Chemical Physics, 1981, 75, 5497-5502.	1.2	16
54	Nonlinear effects in polar fluids: A molecular theory of electrostriction. Journal of Chemical Physics, 1981, 75, 4707-4718.	1.2	40

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55	The adsorption of dipoles at a wall in the presence of an electric field: The RLHNC approximation. Journal of Chemical Physics, 1980, 73, 3980-3986.	1.2	24
56	Monte Carlo study of two ions in a Stockmayer solvent. Faraday Discussions of the Chemical Society, 1977, 64, 22.	2.2	9
57	Computations for Higher Valence Electrolytes in the Restricted Primitive Model. Journal of Chemical Physics, 1972, 56, 3071-3085.	1.2	100
58	Upper bounds on free energies in terms of hard-sphere results. Molecular Physics, 1970, 18, 249-260.	0.8	124
59	Equilibrium Properties of Ionic Solutions; The Primitive Model and its Modification for Aqueous Solutions of the Alkali Halides at 25Â°C. Journal of Chemical Physics, 1970, 52, 704-715.	1.2	74
60	Integral Equation Computations for Aqueous 1â€“1 Electrolytes. Accuracy of the Method. Journal of Chemical Physics, 1969, 50, 3965-3976.	1.2	123
61	Integral Equation Methods in the Computation of Equilibrium Properties of Ionic Solutions. Journal of Chemical Physics, 1968, 48, 2742-2752.	1.2	236