Sukumaran Vasudevan

List of Publications by Year
in descending order

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30 papers	1,567 citations	516561 16 h-index	454834 30 g-index
30 all docs	30 docs citations	30 times ranked	3297 citing authors

#	Article	IF	Citations
1	Ethylene Glycol Dihedral Angle Dynamics: Relating Molecular Conformation to the Raman Spectrum of the Liquid. Journal of Physical Chemistry B, 2021, 125, 1888-1895.	1.2	12
2	Search for H-Bonded Motifs in Liquid Ethylene Glycol Using a Machine Learning Strategy. Journal of Physical Chemistry B, 2021, 125, 5909-5919.	1.2	5
3	Geometry of Hydrogen Bonds in Liquid Ethanol Probed by Proton NMR Experiments. Journal of Physical Chemistry B, 2020, 124, 662-667.	1.2	13
4	Molecular Conformation and Hydrogen Bond Formation in Liquid Ethylene Glycol. Journal of Physical Chemistry B, 2020, 124, 9136-9143.	1.2	8
5	Geometry of OHâ‹¯O interactions in the liquid state of linear alcohols fromab initiomolecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 6690-6697.	1.3	10
6	Hydrogen Bonding in the Liquid State of Linear Alcohols: Molecular Dynamics and Thermodynamics. Journal of Physical Chemistry B, 2020, 124, 3548-3555.	1.2	9
7	The multiple dissociation constants of glutathione disulfide: interpreting experimental pH-titration curves with ab initio MD simulations. Physical Chemistry Chemical Physics, 2019, 21, 9212-9217.	1.3	6
8	Understanding Aqueous Dispersibility of Boron Nitride Nanosheets from 1H Solid State NMR and Reactive Molecular Dynamics. Journal of Physical Chemistry C, 2018, 122, 4662-4669.	1.5	15
9	Grapheneâ€“Solvent Interactions in Nonaqueous Dispersions: 2D ROESY NMR Measurements and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 1881-1888.	1.5	6
10	Distinguishing Intra- and Intermolecular Interactions in Liquid 1,2-Ethanediol by ¹H NMR and Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2018, 122, 9757-9762.	1.2	14
11	Understanding Surfactant Stabilization of MoS₂ Nanosheets in Aqueous Dispersions from Zeta Potential Measurements and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 19243-19250.	1.5	31
12	Conformation of Ethylene Glycol in the Liquid State: Intra- versus Intermolecular Interactions. Journal of Physical Chemistry B, 2017, 121, 5595-5600.	1.2	26
13	Probing Grapheneâ€“Surfactant Interactions in Aqueous Dispersions with Nuclear Overhauser Effect NMR Spectroscopy and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2017, 121, 16637-16643.	1.5	4
14	Liquid-Phase Exfoliation of MoS₂ Nanosheets: The Critical Role of Trace Water. Journal of Physical Chemistry Letters, 2016, 7, 4884-4890.	2.1	101
15	Water Dispersible, Positively and Negatively Charged MoS₂ Nanosheets: Surface Chemistry and the Role of Surfactant Binding. Journal of Physical Chemistry Letters, 2015, 6, 739-744.	2.1	113
16	Estimating successive pK_a values of polyprotic acids from ab initio molecular dynamics using metadynamics: the dissociation of phthalic acid and its isomers. Physical Chemistry Chemical Physics, 2015, 17, 6383-6388.	1.3	37
17	Ab Initio Molecular Dynamics Simulations of Amino Acids in Aqueous Solutions: Estimating pK_a Values from Metadynamics Sampling. Journal of Physical Chemistry B, 2015, 119, 12249-12255.	1.2	27
18	Ab Initio MD Simulations of the BrÃ¸nsted Acidity of Glutathione in Aqueous Solutions: Predicting pK_a Shifts of the Cysteine Residue. Journal of Physical Chemistry B, 2015, 119, 15353-15358.	1.2	40

#	Article	IF	Citations
19	Response to â€œComment on â€˜Communication: Benzene dimerâ€“The free energy landscapeâ€™â€•[J. Chem. Phys. 140, 227101 (2014)]. Journal of Chemical Physics, 2014, 140, 227102.	1.2	2
20	Spectral Migration of Fluorescence in Graphene Oxide Aqueous Dispersions: Evidence for Excited-State Proton Transfer. Journal of Physical Chemistry Letters, 2014, 5, 1-7.	2.1	33
21	Dissociation Constants of Weak Acids from ab Initio Molecular Dynamics Using Metadynamics: Influence of the Inductive Effect and Hydrogen Bonding on pK_a Values. Journal of Physical Chemistry B, 2014, 118, 13651-13657.	1.2	51
22	Glass, Gel, and Liquid Crystals: Arrested States of Graphene Oxide Aqueous Dispersions. Journal of Physical Chemistry C, 2014, 118, 21706-21713.	1.5	48
23	Engineering New Layered Solids from Exfoliated Inorganics: a Periodically Alternating Hydrotalcite â€“ Montmorillonite Layered Hybrid. Scientific Reports, 2013, 3, 3498.	1.6	37
24	Understanding Aqueous Dispersibility of Graphene Oxide and Reduced Graphene Oxide through pK_a Measurements. Journal of Physical Chemistry Letters, 2012, 3, 867-872.	2.1	717
25	Cyclodextrin functionalized magnetic iron oxide nanocrystals: a host-carrier for magnetic separation of non-polar molecules and arsenic from aqueous media. Journal of Materials Chemistry, 2012, 22, 14925.	6.7	53
26	Form, Content, and Magnetism in Iron Oxide Nanocrystals. Journal of Physical Chemistry C, 2011, 115, 18088-18093.	1.5	52
27	Neutral Nanosheets that Gel: Exfoliated Layered Double Hydroxides in Toluene. Journal of Physical Chemistry Letters, 2011, 2, 1193-1198.	2.1	64
28	Spectrally Resolved Resonance Energy Transfer from ZnO:MgO Nanocrystals. Journal of Physical Chemistry C, 2009, 113, 16424-16431.	1.5	12
29	Orientation and Motion of Interlamellar Water:Â An Infrared and NMR Investigation of Water in the Galleries of Layered Cd0.75PS3K0.5(H2O)y. Journal of the American Chemical Society, 2000, 122, 6028-6038.	6.6	17
30	Spin state and exchange in the quasi-one-dimensional antiferromagnet KFeS2. Pramana - Journal of Physics, 1997, 48, 1123-1134.	0.9	4