K Ganapathy Ayappa

List of Publications by Year
in descending order

72	1,948	218677	289244
papers	citations	26 h-index	40 g-index

81	81	81	1727
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Analysis of microwave sintering of ceramics. AICHE Journal, 1998, 44, 2302-2311.	3.6	110
2	Influence of internal convection during microwave thawing of cylinders. AICHE Journal, 2001, 47, 835-850.	3.6	86
3	Analysis of microwave thawing of slabs with effective heat capacity method. AICHE Journal, 1997, 43, 1662-1674.	3.6	85
4	Adsorption Isotherms of Water on Mica: Redistribution and Film Growth. Journal of Physical Chemistry B, 2009, 113, 1058-1067.	2.6	83
5	Influence of Hydrophilic Surface Specificity on the Structural Properties of Confined Water. Journal of Physical Chemistry B, 2009, 113, 13825-13839.	2.6	80
6	Entropy and dynamics of water in hydration layers of a bilayer. Journal of Chemical Physics, 2010, 133, 174704.	3.0	79
7	The structure of frozen phases in slit nanopores: A grand canonical Monte Carlo study. Journal of Chemical Physics, 2002, 117, 5373-5383.	3.0	62
8	Resonant microwave power absorption in slabs and cylinders. AICHE Journal, 1997, 43, 615-624.	3.6	59
9	Simulations of Binary Mixture Adsorption in Carbon Nanotubes:Â Transitions in Adsorbed Fluid Composition. Langmuir, 1998, 14, 880-890.	3.5	57
10	Cholesterol promotes Cytolysin A activity by stabilizing the intermediates during pore formation. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7323-E7330.	7.1	48
11	Power Absorption During Microwave Heating of Emulsions and Layered Systems. Journal of Food Science, 1995, 60, 1132-1136.	3.1	46
12	Enhanced Gas Adsorption on Graphitic Substrates via Defects and Local Curvature: A Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 7741-7750.	3.1	43
13	Super-resolution Stimulated Emission Depletion-Fluorescence Correlation Spectroscopy Reveals Nanoscale Membrane Reorganization Induced by Pore-Forming Proteins. Langmuir, 2016, 32, 9649-9657.	3.5	43
14	Freezing of Fluids Confined between Mica Surfaces. Journal of Physical Chemistry B, 2007, 111, 14299-14310.	2.6	39
15	Microwave driven convection in a square cavity. AICHE Journal, 1994, 40, 1268-1272.	3.6	37
16	Modeling velocity autocorrelation functions of confined fluids: A memory function approach. Journal of Chemical Physics, 2003, 118, 690-705.	3.0	37
17	Filling Characteristics for an Activated Carbon Based Adsorbed Natural Gas Storage System. Industrial & Engineering Chemistry Research, 2011, 50, 13000-13011.	3.7	37
18	Relaxation and jump dynamics of water at the mica interface. Journal of Chemical Physics, 2012, 136, 194701.	3.0	37

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19	Correlated protein conformational states and membrane dynamics during attack by pore-forming toxins. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 12839-12844.	7.1	34
20	Developing a Coarse-Grained Model for Bacterial Cell Walls: Evaluating Mechanical Properties and Free Energy Barriers. Journal of Chemical Theory and Computation, 2020, 16, 5369-5384.	5.3	31
21	The Influence of Bilayer Composition on the Gel to Liquid Crystalline Transition. Journal of Physical Chemistry B, 2009, 113, 10660-10668.	2.6	30
22	Adsorption on Edge-Functionalized Bilayer Graphene Nanoribbons: Assessing the Role of Functional Groups in Methane Uptake. Journal of Physical Chemistry C, 2012, 116, 23394-23403.	3.1	30
23	Evaluating methane storage targets: from powder samples to onboard storage systems. Adsorption, 2014, 20, 769-776.	3.0	30
24	Capturing the Membrane-Triggered Conformational Transition of an Î±-Helical Pore-Forming Toxin. Journal of Physical Chemistry B, 2016, 120, 12064-12078.	2.6	30
25	Molecular Dynamics Study of the Structure, Flexibility, and Hydrophilicity of PETIM Dendrimers: A Comparison with PAMAM Dendrimers. Journal of Physical Chemistry B, 2015, 119, 12990-13001.	2.6	29
26	Estimation of activation energy for electroporation and pore growth rate in liquid crystalline and gel phases of lipid bilayers using molecular dynamics simulations. Soft Matter, 2015, 11, 8632-8640.	2.7	29
27	Assessing Barriers for Antimicrobial Penetration in Complex Asymmetric Bacterial Membranes: A Case Study with Thymol. Langmuir, 2020, 36, 8800-8814.	3.5	29
28	Density distributions of diatoms in carbon nanotubes: A grand canonical Monte Carlo study. Journal of Chemical Physics, 1998, 109, 4576-4586.	3.0	27
29	Non-monotonic, distance-dependent relaxation of water in reverse micelles: Propagation of surface induced frustration along hydrogen bond networks. Journal of Chemical Physics, 2012, 137, 014515.	3.0	27
30	Lysis dynamics and membrane oligomerization pathways for Cytolysin A (ClyA) pore-forming toxin. RSC Advances, 2014, 4, 4930.	3.6	27
31	A new microscopic insight into membrane penetration and reorganization by PETIM dendrimers. Soft Matter, 2014, 10, 7577-7587.	2.7	27
32	Effect of Polymer Grafting on the Bilayer Gel to Liquid-Crystalline Transition. Journal of Physical Chemistry B, 2010, 114, 2738-2748.	2.6	25
33	Assessing the Structure and Stability of Transmembrane Oligomeric Intermediates of an Î±-Helical Toxin. Langmuir, 2017, 33, 11496-11510.	3.5	25
34	Verifying scalings for bending rigidity of bilayer membranes using mesoscale models. Soft Matter, 2011, 7, 3963.	2.7	24
35	Enhancing the Dynamics of Water Confined between Graphene Oxide Surfaces with Janus Interfaces: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2019, 123, 2978-2993.	2.6	24
36	Complex dynamics at the nanoscale in simple biomembranes. Scientific Reports, 2017, 7, 11173.	3.3	23

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37	Solvation force, structure and thermodynamics of fluids confined in geometrically rough pores. Journal of Chemical Physics, 2004, 120, 9703-9714.	3.0	22
38	Laterally structured ripple and square phases with one and two dimensional thickness modulations in a model bilayer system. Soft Matter, 2014, 10, 7630-7637.	2.7	22
39	Dendrimer Interactions with Lipid Bilayer: Comparison of Force Field and Effect of Implicit vs Explicit Solvation. Journal of Chemical Theory and Computation, 2018, 14, 3825-3839.	5.3	21
40	Nanoscale dynamics of phospholipids reveals an optimal assembly mechanism of pore-forming proteins in bilayer membranes. Physical Chemistry Chemical Physics, 2016, 18, 29935-29945.	2.8	20
41	Molecular Dynamics Study of Lipid and Cholesterol Reorganization Due to Membrane Binding and Pore Formation by Listeriolysin O. Journal of Membrane Biology, 2020, 253, 535-550.	2.1	20
42	Glassy dynamics in a confined monatomic fluid. Physical Review E, 2012, 86, 011504.	2.1	19
43	pH controlled gating of toxic protein pores by dendrimers. Nanoscale, 2016, 8, 13045-13058.	5.6	18
44	Comparison of coarse-grained (MARTINI) and atomistic molecular dynamics simulations of $$alpha $$ Î± and $$eta $$ Î² toxin nanopores in lipid membranes. Journal of Chemical Sciences, 2017, 129, 1017-1030.	1.5	18
45	The Solvent-Exposed C-Terminus of the Cytolysin A Pore-Forming Toxin Directs Pore Formation and Channel Function in Membranes. Biochemistry, 2016, 55, 5952-5961.	2.5	17
46	Transmembrane oligomeric intermediates of pore forming toxin Cytolysin A determine leakage kinetics. RSC Advances, 2017, 7, 51750-51762.	3.6	15
47	Mechanistic Insights into Pore Formation by an Î±-Pore Forming Toxin: Protein and Lipid Bilayer Interactions of Cytolysin A. Accounts of Chemical Research, 2021, 54, 120-131.	15.6	14
48	Distinct Diffusion in Binary Mixtures Confined in Slit Graphite Pores. Journal of Physical Chemistry B, 2004, 108, 4411-4421.	2.6	13
49	Assessing the extent of the structural and dynamic modulation of membrane lipids due to pore forming toxins: insights from molecular dynamics simulations. Soft Matter, 2020, 16, 4840-4857.	2.7	13
50	Opening of smaller toxin pores by lipid micelle formation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5107-5108.	7.1	12
51	Statistical thermodynamics of lattice models in zeolites: Implications of local versus global mean field interactions. Journal of Chemical Physics, 1999, 111, 4736-4742.	3.0	10
52	Influence of surface commensurability on the structure and relaxation dynamics of a confined monatomic fluid. Journal of Chemical Physics, 2018, 149, 064503.	3.0	10
53	Structural Transitions of Nitrogen Confined in Slit Graphite Pores. Langmuir, 2001, 17, 5245-5255.	3.5	9
54	Structure and Dynamics of Octamethylcyclotetrasiloxane Confined between Mica Surfaces. Journal of Physical Chemistry B, 2016, 120, 2951-2967.	2.6	9

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55	Using multiscale molecular dynamics simulations to obtain insights into pore forming toxin mechanisms. Methods in Enzymology, 2021, 649, 461-502.	1.0	9
56	Pore Forming Protein Induced Biomembrane Reorganization and Dynamics: A Focused Review. Frontiers in Molecular Biosciences, 2021, 8, 737561.	3.5	9
57	Melting and mechanical properties of polymer grafted lipid bilayer membranes. Journal of Chemical Physics, 2011, 135, 104901.	3.0	7
58	Dynamical Transitions of Supercooled Water in Graphene Oxide Nanopores: Influence of Surface Hydrophilicity. Journal of Physical Chemistry B, 2020, 124, 4805-4820.	2.6	7
59	Influence of the extent of hydrophobicity on water organization and dynamics on 2D graphene oxide surfaces. Physical Chemistry Chemical Physics, 2022, 24, 14909-14923.	2.8	7
60	Combined Atomic Force Microscopy and Modeling Study of The Evolution of Octadecylamine Films on a Mica Surface. Journal of Physical Chemistry C, 2010, 114, 3549-3559.	3.1	6
61	Confined fluids in a Janus pore: influence of surface asymmetry on structure and solvation forces. Molecular Simulation, 2012, 38, 1114-1123.	2.0	6
62	Influence of surface hydrophilicity and hydration on the rotational relaxation of supercooled water on graphene oxide surfaces. Physical Chemistry Chemical Physics, 2020, 22, 16080-16095.	2.8	6
63	Predicting interfacial hot-spot residues that stabilize protein-protein interfaces in oligomeric membrane-toxin pores through hydrogen bonds and salt bridges. Journal of Biomolecular Structure and Dynamics, 2021, 39, 20-34.	3.5	6
64	Evaluating Coarse-Grained MARTINI Force-Fields for Capturing the Ripple Phase of Lipid Membranes. Journal of Physical Chemistry B, 2021, 125, 6587-6599.	2.6	6
65	A generic force field for simulating native protein structures using dissipative particle dynamics. Soft Matter, 2021, 17, 9772-9785.	2.7	6
66	Model for dynamics of inhomogeneous and bulk fluids. Journal of Chemical Physics, 2006, 124, 144503.	3.0	4
67	Hydrophobic Gating and 1/f Noise of the Anthrax Toxin Channel. Journal of Physical Chemistry B, 2021, 125, 5466-5478.	2.6	4
68	Bacterial protein listeriolysin O induces nonmonotonic dynamics because of lipid ejection and crowding. Biophysical Journal, 2021, 120, 3040-3049.	0.5	4
69	Self-diffusivity and velocity autocorrelation functions for xenon in NaY using memory kernels. Molecular Physics, 2006, 104, 3809-3819.	1.7	3
70	Coupling of mitochondrial population evolution to microtubule dynamics in fission yeast cells: a kinetic Monte Carlo study. Soft Matter, 2022, 18, 4483-4492.	2.7	2
71	Molecular dynamics study of vacancy diffusion in a forced Lennard-Jones system. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2000, 80, 301-310.	0.6	1
72	Physical understanding of pore formation on supported lipid bilayer by bacterial toxins. , 2013, , .		0