# 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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | Using multiscale molecular dynamics simulations to obtain insights into pore forming toxin mechanisms. Methods in Enzymology, 2021, 649, 461-502. | 1.0 | 9 |
| 5 | Hydrophobic Gating and 1/f Noise of the Anthrax Toxin Channel. Journal of Physical Chemistry B, 2021, 125, 5466-5478. | 2.6 | 4 |
| 6 | 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 |
| 7 | Bacterial protein listeriolysin O induces nonmonotonic dynamics because of lipid ejection and crowding. Biophysical Journal, 2021, 120, 3040-3049. | 0.5 | 4 |
| 8 | Pore Forming Protein Induced Biomembrane Reorganization and Dynamics: A Focused Review. Frontiers in Molecular Biosciences, 2021, 8, 737561. | 3.5 | 9 |
| 9 | A generic force field for simulating native protein structures using dissipative particle dynamics. Soft Matter, 2021, 17, 9772-9785. | 2.7 | 6 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | Assessing Barriers for Antimicrobial Penetration in Complex Asymmetric Bacterial Membranes: A Case Study with Thymol. Langmuir, 2020, 36, 8800-8814. | 3.5 | 29 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

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|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |
| 23 | Assessing the Structure and Stability of Transmembrane Oligomeric Intermediates of an Î±-Helical Toxin. Langmuir, 2017, 33, 11496-11510. | 3.5 | 25 |
| 24 | Complex dynamics at the nanoscale in simple biomembranes. Scientific Reports, 2017, 7, 11173. | 3.3 | 23 |
| 25 | Transmembrane oligomeric intermediates of pore forming toxin Cytolysin A determine leakage kinetics. RSC Advances, 2017, 7, 51750-51762. | 3.6 | 15 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | 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 |
| 30 | 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 |
| 31 | pH controlled gating of toxic protein pores by dendrimers. Nanoscale, 2016, 8, 13045-13058. | 5.6 | 18 |
| 32 | Structure and Dynamics of Octamethylcyclotetrasiloxane Confined between Mica Surfaces. Journal of Physical Chemistry B, 2016, 120, 2951-2967. | 2.6 | 9 |
| 33 | 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 |
| 34 | 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 |
| 35 | Lysis dynamics and membrane oligomerization pathways for Cytolysin A (ClyA) pore-forming toxin. RSC Advances, 2014, 4, 4930. | 3.6 | 27 |
| 36 | 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 |

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| 37 | A new microscopic insight into membrane penetration and reorganization by PETIM dendrimers. Soft Matter, 2014, 10, 7577-7587. | 2.7 | 27 |
| 38 | Evaluating methane storage targets: from powder samples to onboard storage systems. Adsorption, 2014, 20, 769-776. | 3.0 | 30 |
| 39 | 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 |
| 40 | Physical understanding of pore formation on supported lipid bilayer by bacterial toxins. , 2013, , . | | 0 |
| 41 | Relaxation and jump dynamics of water at the mica interface. Journal of Chemical Physics, 2012, 136, 194701. | 3.0 | 37 |
| 42 | 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 |
| 43 | 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 |
| 44 | Confined fluids in a Janus pore: influence of surface asymmetry on structure and solvation forces. Molecular Simulation, 2012, 38, 1114-1123. | 2.0 | 6 |
| 45 | Glassy dynamics in a confined monatomic fluid. Physical Review E, 2012, 86, 011504. | 2.1 | 19 |
| 46 | Verifying scalings for bending rigidity of bilayer membranes using mesoscale models. Soft Matter, 2011, 7, 3963. | 2.7 | 24 |
| 47 | Filling Characteristics for an Activated Carbon Based Adsorbed Natural Gas Storage System. Industrial & Engineering Chemistry Research, 2011, 50, 13000-13011. | 3.7 | 37 |
| 48 | Melting and mechanical properties of polymer grafted lipid bilayer membranes. Journal of Chemical Physics, 2011, 135, 104901. | 3.0 | 7 |
| 49 | Effect of Polymer Grafting on the Bilayer Gel to Liquid-Crystalline Transition. Journal of Physical Chemistry B, 2010, 114, 2738-2748. | 2.6 | 25 |
| 50 | 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 |
| 51 | Entropy and dynamics of water in hydration layers of a bilayer. Journal of Chemical Physics, 2010, 133, 174704. | 3.0 | 79 |
| 52 | Adsorption Isotherms of Water on Mica: Redistribution and Film Growth. Journal of Physical Chemistry B, 2009, 113, 1058-1067. | 2.6 | 83 |
| 53 | The Influence of Bilayer Composition on the Gel to Liquid Crystalline Transition. Journal of Physical Chemistry B, 2009, 113, 10660-10668. | 2.6 | 30 |
| 54 | Influence of Hydrophilic Surface Specificity on the Structural Properties of Confined Water. Journal of Physical Chemistry B, 2009, 113, 13825-13839. | 2.6 | 80 |

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| 55 | Freezing of Fluids Confined between Mica Surfaces. Journal of Physical Chemistry B, 2007, 111, 14299-14310. | 2.6 | 39 |
| 56 | Self-diffusivity and velocity autocorrelation functions for xenon in NaY using memory kernels. Molecular Physics, 2006, 104, 3809-3819. | 1.7 | 3 |
| 57 | Model for dynamics of inhomogeneous and bulk fluids. Journal of Chemical Physics, 2006, 124, 144503. | 3.0 | 4 |
| 58 | Solvation force, structure and thermodynamics of fluids confined in geometrically rough pores. Journal of Chemical Physics, 2004, 120, 9703-9714. | 3.0 | 22 |
| 59 | Distinct Diffusion in Binary Mixtures Confined in Slit Graphite Pores. Journal of Physical Chemistry B, 2004, 108, 4411-4421. | 2.6 | 13 |
| 60 | Modeling velocity autocorrelation functions of confined fluids: A memory function approach. Journal of Chemical Physics, 2003, 118, 690-705. | 3.0 | 37 |
| 61 | 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 |
| 62 | Structural Transitions of Nitrogen Confined in Slit Graphite Pores. Langmuir, 2001, 17, 5245-5255. | 3.5 | 9 |
| 63 | Influence of internal convection during microwave thawing of cylinders. AICHE Journal, 2001, 47, 835-850. | 3.6 | 86 |
| 64 | 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 |
| 65 | 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 |
| 66 | Analysis of microwave sintering of ceramics. AICHE Journal, 1998, 44, 2302-2311. | 3.6 | 110 |
| 67 | Simulations of Binary Mixture Adsorption in Carbon Nanotubes:Â Transitions in Adsorbed Fluid Composition. Langmuir, 1998, 14, 880-890. | 3.5 | 57 |
| 68 | Density distributions of diatoms in carbon nanotubes: A grand canonical Monte Carlo study. Journal of Chemical Physics, 1998, 109, 4576-4586. | 3.0 | 27 |
| 69 | Resonant microwave power absorption in slabs and cylinders. AICHE Journal, 1997, 43, 615-624. | 3.6 | 59 |
| 70 | Analysis of microwave thawing of slabs with effective heat capacity method. AICHE Journal, 1997, 43, 1662-1674. | 3.6 | 85 |
| 71 | Power Absorption During Microwave Heating of Emulsions and Layered Systems. Journal of Food Science, 1995, 60, 1132-1136. | 3.1 | 46 |
| 72 | Microwave driven convection in a square cavity. AICHE Journal, 1994, 40, 1268-1272. | 3.6 | 37 |