Hwankyu Lee

List of Publications by Year
in descending order

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76 papers	3,386 citations	249298 26 h-index	162838 57 g-index
77 all docs	77 docs citations	77 times ranked	5320 citing authors

#	Article	IF	Citations
1	Mechanistic Pathway of Lipid Phase-Dependent Lipid Corona Formation on Phenylalanine-Functionalized Gold Nanoparticles: A Combined Experimental and Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2022, 126, 2241-2255.	1.2	7
2	Topological analysis of single-stranded DNA with an alpha-hederin nanopore. Biosensors and Bioelectronics, 2021, 171, 112711.	5.3	3
3	Effect of Protein Corona on Nanoparticleâ€“Lipid Membrane Binding: The Binding Strength and Dynamics. Langmuir, 2021, 37, 3751-3760.	1.6	8
4	Allâ€Atom Simulations and Freeâ€Energy Calculations of Antibodies Bound to the Spike Protein of SARSâ€CoVâ€2: The Binding Strength and Multivalent Hydrogenâ€Bond Interactions. Advanced Theory and Simulations, 2021, 4, 2100012.	1.3	2
5	Reverse Actuation of Polyelectrolyte Effect for In Vivo Antifouling. ACS Nano, 2021, 15, 6811-6828.	7.3	30
6	Molecular Modeling of Protein Corona Formation and Its Interactions with Nanoparticles and Cell Membranes for Nanomedicine Applications. Pharmaceutics, 2021, 13, 637.	2.0	15
7	Multivalent Nanosheet Antibody Mimics for Selective Microbial Recognition and Inactivation. Advanced Materials, 2021, 33, e2101376.	11.1	8
8	Antibacterial Strategies: Multivalent Nanosheet Antibody Mimics for Selective Microbial Recognition and Inactivation (Adv. Mater. 22/2021). Advanced Materials, 2021, 33, 2170173.	11.1	0
9	Transition-Metal Dichalcogenide Artificial Antibodies with Multivalent Polymeric Recognition Phases for Rapid Detection and Inactivation of Pathogens. Journal of the American Chemical Society, 2021, 143, 14635-14645.	6.6	17
10	A simple strategy for signal enhancement in lateral flow assays using superabsorbent polymers. Mikrochimica Acta, 2021, 188, 364.	2.5	1
11	Supramolecular Functionalization for Improving Thermoelectric Properties of Single-Walled Carbon Nanotubesâ€“Small Organic Molecule Hybrids. ACS Applied Materials & Interfaces, 2020, 12, 51387-51396.	4.0	13
12	Molecular Simulations of PEGylated Biomolecules, Liposomes, and Nanoparticles for Drug Delivery Applications. Pharmaceutics, 2020, 12, 533.	2.0	38
13	Corona Formation: Effects of Nanoparticle Electrostatics and Proteinâ€“Protein Interactions on Corona Formation: Conformation and Hydrodynamics (Small 10/2020). Small, 2020, 16, 2070054.	5.2	5
14	Supramolecular Assemblies: Supramolecular Protein Assembly Retains Its Structural Integrity at Liquidâ€“Liquid Interface (Adv. Mater. Interfaces 4/2020). Advanced Materials Interfaces, 2020, 7, 2070021.	1.9	1
15	Quantitative Interpretation of Hydration Dynamics Enabled the Fabrication of a Zwitterionic Antifouling Surface. ACS Applied Materials & Interfaces, 2020, 12, 7951-7965.	4.0	38
16	Supramolecular Protein Assembly Retains Its Structural Integrity at Liquidâ€“Liquid Interface. Advanced Materials Interfaces, 2020, 7, 1901674.	1.9	4
17	Effects of Nanoparticle Electrostatics and Proteinâ€“Protein Interactions on Corona Formation: Conformation and Hydrodynamics. Small, 2020, 16, e1906598.	5.2	37
18	Heterodimer and pore formation of magainin 2 and PGLa: The anchoring and tilting of peptides in lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183305.	1.4	6

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19	Self-assembled DNA hollow spheres from microsponges. Biofabrication, 2019, 11, 025016.	3.7	3
20	Effects of hydrophobic and hydrogen-bond interactions on the binding affinity of antifreeze proteins to specific ice planes. Journal of Molecular Graphics and Modelling, 2019, 87, 48-55.	1.3	9
21	Alpha-Hederin Nanopore for Single Nucleotide Discrimination. ACS Nano, 2019, 13, 1719-1727.	7.3	11
22	Effect of low levels of lipid oxidation on the curvature, dynamics, and permeability of lipid bilayers and their interactions with cationic nanoparticles. Journal Physics D: Applied Physics, 2018, 51, 164002.	1.3	13
23	Disassembly and trimer formation of E2 protein cage: the effects of C-terminus, salt, and protonation state. Journal Physics D: Applied Physics, 2018, 51, 365402.	1.3	0
24	Structures, dynamics, and hydrogen-bond interactions of antifreeze proteins in TIP4P/Ice water and their dependence on force fields. PLoS ONE, 2018, 13, e0198887.	1.1	20
25	Cytoprotective Self-assembled RGD Peptide Nanofilms for Surface Modification of Viable Mesenchymal Stem Cells. Chemistry of Materials, 2017, 29, 2055-2065.	3.2	51
26	Aggregation and insertion of melittin and its analogue MelP5 into lipid bilayers at different concentrations: effects on pore size, bilayer thickness and dynamics. Physical Chemistry Chemical Physics, 2017, 19, 7195-7203.	1.3	17
27	Adsorption of plasma proteins onto PEGylated single-walled carbon nanotubes: The effects of protein shape, PEG size and grafting density. Journal of Molecular Graphics and Modelling, 2017, 75, 1-8.	1.3	11
28	Effects of the asphaltene structure and the tetralin/heptane solvent ratio on the size and shape of asphaltene aggregates. Physical Chemistry Chemical Physics, 2017, 19, 13931-13940.	1.3	16
29	Multilayer Nanofilms via Inkjet Printing for Stabilizing Growth Factor and Designing Desired Cell Developments. Advanced Healthcare Materials, 2017, 6, 1700216.	3.9	8
30	Beneficial roles of H-donors as diluent and H-shuttle for asphaltenes in catalytic upgrading of vacuum residue. Chemical Engineering Journal, 2017, 314, 1-10.	6.6	41
31	In vitro blood cell viability profiling of polymers used in molecular assembly. Scientific Reports, 2017, 7, 9481.	1.6	76
32	Effect of lipid shape on toroidal pore formation and peptide orientation in lipid bilayers. Physical Chemistry Chemical Physics, 2017, 19, 21340-21349.	1.3	14
33	Modulation of the Vault Protein-Protein Interaction for Tuning of Molecular Release. Scientific Reports, 2017, 7, 14816.	1.6	8
34	Effect of polyelectrolyte size on multilayer conformation and dynamics at different temperatures and salt concentrations. Journal of Molecular Graphics and Modelling, 2016, 70, 246-252.	1.3	17
35	All-atom simulations and free-energy calculations of coiled-coil peptides with lipid bilayers: binding strength, structural transition, and effect on lipid dynamics. Scientific Reports, 2016, 6, 22299.	1.6	17
36	Adsorption of Plasma Proteins onto PEGylated Lipid Bilayers: The Effect of PEG Size and Grafting Density. Biomacromolecules, 2016, 17, 1757-1765.	2.6	75

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37	Effects of temperature, salt concentration, and the protonation state on the dynamics and hydrogen-bond interactions of polyelectrolyte multilayers on lipid membranes. Physical Chemistry Chemical Physics, 2016, 18, 6691-6700.	1.3	15
38	The binding and insertion of imidazolium-based ionic surfactants into lipid bilayers: the effects of the surfactant size and salt concentration. Physical Chemistry Chemical Physics, 2015, 17, 5725-5733.	1.3	18
39	Effects of imidazolium-based ionic surfactants on the size and dynamics of phosphatidylcholine bilayers with saturated and unsaturated chains. Journal of Molecular Graphics and Modelling, 2015, 60, 162-168.	1.3	7
40	Effects of imidazolium-based ionic liquids on the stability and dynamics of gramicidin A and lipid bilayers at different salt concentrations. Journal of Molecular Graphics and Modelling, 2015, 61, 53-60.	1.3	18
41	Design of a reversible inversed pH-responsive caged protein. Biomaterials Science, 2015, 3, 627-635.	2.6	9
42	Investigation of Ion Channel Activities of Gramicidin A in the Presence of Ionic Liquids Using Model Cell Membranes. Scientific Reports, 2015, 5, 11935.	1.6	24
43	Structural effects of tachyplesin I and its linear derivative on their aggregation and mobility in lipid bilayers. Journal of Molecular Graphics and Modelling, 2015, 59, 123-128.	1.3	11
44	Synergistic effects of magainin 2 and PGLa on their heterodimer formation, aggregation, and insertion into the bilayer. RSC Advances, 2015, 5, 2047-2055.	1.7	27
45	Dispersion and bilayer interaction of single-walled carbon nanotubes modulated by covalent and noncovalent PEGylation. Molecular Simulation, 2015, 41, 1254-1263.	0.9	10
46	Molecular Modeling of PEGylated Peptides, Dendrimers, and Single-Walled Carbon Nanotubes for Biomedical Applications. Polymers, 2014, 6, 776-798.	2.0	34
47	Dynamics and stability of lipid bilayers modulated by thermosensitive polypeptides, cholesterols, and PEGylated lipids. Physical Chemistry Chemical Physics, 2014, 16, 3763.	1.3	15
48	Effect of the structural difference between Bax-Î±5 and Bcl-xL-Î±5 on their interactions with lipid bilayers. Physical Chemistry Chemical Physics, 2014, 16, 981-988.	1.3	6
49	Molecular Dynamics Studies of PEGylated Î±-Helical Coiled Coils and Their Self-Assembled Micelles. Langmuir, 2014, 30, 8848-8855.	1.6	20
50	Formulation Optimization and In Vivo Proof-of-Concept Study of Thermosensitive Liposomes Balanced by Phospholipid, Elastin-Like Polypeptide, and Cholesterol. PLoS ONE, 2014, 9, e103116.	1.1	20
51	Molecular Dynamics Studies of PEGylated Single-Walled Carbon Nanotubes: The Effect of PEG Size and Grafting Density. Journal of Physical Chemistry C, 2013, 117, 26334-26341.	1.5	32
52	Effects of PEGylation on the Binding Interaction of Magainin 2 and Tachyplesin I with Lipid Bilayer Surface. Langmuir, 2013, 29, 14214-14221.	1.6	31
53	Membrane penetration and curvature induced by single-walled carbon nanotubes: the effect of diameter, length, and concentration. Physical Chemistry Chemical Physics, 2013, 15, 16334.	1.3	11
54	Effect of peptide conformation on TiO2 biomineralization. Dalton Transactions, 2013, 42, 13817.	1.6	11

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55	Interparticle Dispersion, Membrane Curvature, and Penetration Induced by Single-Walled Carbon Nanotubes Wrapped with Lipids and PEGylated Lipids. Journal of Physical Chemistry B, 2013, 117, 1337-1344.	1.2	26
56	Effect of Arginine-Rich Peptide Length on the Structure and Binding Strength of siRNAâ€“Peptide Complexes. Journal of Physical Chemistry B, 2013, 117, 6917-6926.	1.2	18
57	Effects of the Size, Shape, and Structural Transition of Thermosensitive Polypeptides on the Stability of Lipid Bilayers and Liposomes. Macromolecules, 2012, 45, 7304-7312.	2.2	16
58	Isolating a Trimer Intermediate in the Self-Assembly of E2 Protein Cage. Biomacromolecules, 2012, 13, 699-705.	2.6	19
59	Self-assembly of mixtures of a dendrimer and lipids: effects of hydrophobicity and electrostatics. Molecular Simulation, 2012, 38, 534-539.	0.9	5
60	Self-Assembly of Lipids and Single-Walled Carbon Nanotubes: Effects of Lipid Structure and PEGylation. Journal of Physical Chemistry C, 2012, 116, 9327-9333.	1.5	41
61	Effects of salt on the size and internal structure of PAMAM dendrimers at different pH. Molecular Simulation, 2012, 38, 589-594.	0.9	4
62	Molecular Dynamics Studies of the Size and Internal Structure of the PAMAM Dendrimer Grafted with Arginine and Histidine. Macromolecules, 2011, 44, 8681-8686.	2.2	30
63	Membrane Pore Formation Induced by Acetylated and Polyethylene Glycol-Conjugated Polyamidoamine Dendrimers. Journal of Physical Chemistry C, 2011, 115, 5316-5322.	1.5	39
64	Coarse-Grained Model for PEGylated Lipids: Effect of PEGylation on the Size and Shape of Self-Assembled Structures. Journal of Physical Chemistry B, 2011, 115, 7830-7837.	1.2	104
65	Effects of PEGylation on the Size and Internal Structure of Dendrimers: Self-Penetration of Long PEG Chains into the Dendrimer Core. Macromolecules, 2011, 44, 2291-2298.	2.2	82
66	Multiscale Modeling of Dendrimers and Their Interactions with Bilayers and Polyelectrolytes. Molecules, 2009, 14, 423-438.	1.7	82
67	Molecular Dynamics Study of the Structure and Interparticle Interactions of Polyethylene Glycol-Conjugated PAMAM Dendrimers. Journal of Physical Chemistry B, 2009, 113, 13202-13207.	1.2	60
68	A Coarse-Grained Model for Polyethylene Oxide and Polyethylene Glycol: Conformation and Hydrodynamics. Journal of Physical Chemistry B, 2009, 113, 13186-13194.	1.2	338
69	Structure and Dynamics of Helix-0 of the N-BAR Domain in Lipid Micelles and Bilayers. Biophysical Journal, 2008, 95, 4315-4323.	0.2	47
70	Coarse-Grained Molecular Dynamics Studies of the Concentration and Size Dependence of Fifth- and Seventh-Generation PAMAM Dendrimers on Pore Formation in DMPC Bilayer. Journal of Physical Chemistry B, 2008, 112, 7778-7784.	1.2	155
71	Molecular Dynamics Studies of Polyethylene Oxide and Polyethylene Glycol: Hydrodynamic Radius and Shape Anisotropy. Biophysical Journal, 2008, 95, 1590-1599.	0.2	415
72	Lipid Bilayer Curvature and Pore Formation Induced by Charged Linear Polymers and Dendrimers: The Effect of Molecular Shape. Journal of Physical Chemistry B, 2008, 112, 12279-12285.	1.2	106

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73	Molecular Dynamics Simulations of PAMAM Dendrimer-Induced Pore Formation in DPPC Bilayers with a Coarse-Grained Model. Journal of Physical Chemistry B, 2006, 110, 18204-18211.	1.2	196
74	Molecular Dynamics Studies of the Size, Shape, and Internal Structure of 0% and 90% Acetylated Fifth-Generation Polyamidoamine Dendrimers in Water and Methanol. Journal of Physical Chemistry B, 2006, 110, 4014-4019.	1.2	85
75	The centrosomal protein nephrocystin-6 is mutated in Joubert syndrome and activates transcription factor ATF4. Nature Genetics, 2006, 38, 674-681.	9.4	535
76	Molecular Dynamics Simulations of the Anchoring and Tilting of the Lung-Surfactant Peptide SP-B1-25 in Palmitic Acid Monolayers. Biophysical Journal, 2005, 89, 3807-3821.	0.2	21