Albert J Markvoort

List of Publications by Year
in descending order

69 papers	4,119 citations	126907 33 h-index	114465 63 g-index
80 all docs	80 docs citations	80 times ranked	4386 citing authors

#	Article	IF	Citations
1	Pathway complexity in supramolecular polymerization. Nature, 2012, 481, 492-496.	27.8	812
2	Non-equilibrium supramolecular polymerization. Chemical Society Reviews, 2017, 46, 5476-5490.	38.1	429
3	Mechanism and microkinetics of the Fischerâ€“Tropsch reaction. Physical Chemistry Chemical Physics, 2013, 15, 17038.	2.8	233
4	Theoretical models of nonlinear effects in two-component cooperative supramolecular copolymerizations. Nature Communications, 2011, 2, 509.	12.8	184
5	An Equilibrium Model for Chiral Amplification in Supramolecular Polymers. Journal of Physical Chemistry B, 2012, 116, 5291-5301.	2.6	175
6	Programmable chemical reaction networks: emulating regulatory functions in living cells using a bottom-up approach. Chemical Society Reviews, 2015, 44, 7465-7483.	38.1	123
7	Competing Interactions in Hierarchical Porphyrin Self-Assembly Introduce Robustness in Pathway Complexity. Journal of the American Chemical Society, 2018, 140, 7810-7819.	13.7	123
8	Supramolecular Block Copolymers under Thermodynamic Control. Journal of the American Chemical Society, 2018, 140, 7168-7175.	13.7	119
9	A Detailed Look at Vesicle Fusion. Journal of Physical Chemistry B, 2006, 110, 13212-13219.	2.6	103
10	Kinetic Analysis as a Tool to Distinguish Pathway Complexity in Molecular Assembly: An Unexpected Outcome of Structures in Competition. Journal of the American Chemical Society, 2015, 137, 12677-12688.	13.7	92
11	Unexpectedly Strong Chiral Amplification of Chiral/Achiral and Chiral/Chiral Copolymers of Biphenylylacetylenes and Further Enhancement/Inversion and Memory of the Macromolecular Helicity. Journal of the American Chemical Society, 2019, 141, 7605-7614.	13.7	92
12	Molecular dynamics study of the influence of wall-gas interactions on heat flow in nanochannels. Physical Review E, 2005, 71, 066702.	2.1	82
13	The Bilayerâ^'Vesicle Transition Is Entropy Driven. Journal of Physical Chemistry B, 2005, 109, 22649-22654.	2.6	80
14	Computation of accommodation coefficients and the use of velocity correlation profiles in molecular dynamics simulations. Physical Review E, 2010, 81, 011203.	2.1	72
15	Supramolecular Copolymers: Structure and Composition Revealed by Theoretical Modeling. Journal of the American Chemical Society, 2017, 139, 7036-7044.	13.7	64
16	Vesicle Shapes from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 22780-22785.	2.6	62
17	Proximity-induced caspase-9 activation on a DNA origami-based synthetic apoptosome. Nature Catalysis, 2020, 3, 295-306.	34.4	62
18	Lipid Acrobatics in the Membrane Fusion Arena. Current Topics in Membranes, 2011, 68, 259-294.	0.9	60

#	Article	IF	Citations
19	Model-driven optimization of multicomponent self-assembly processes. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17205-17210.	7.1	57
20	Kinetics of the Fischerâ€“Tropsch Reaction. Angewandte Chemie - International Edition, 2012, 51, 9015-9019.	13.8	55
21	Monomer Formation Model versus Chain Growth Model of the Fischerâ€“Tropsch Reaction. Journal of Physical Chemistry C, 2013, 117, 4488-4504.	3.1	55
22	Lipid-Based Mechanisms for Vesicle Fission. Journal of Physical Chemistry B, 2007, 111, 5719-5725.	2.6	54
23	Tuning the Length of Cooperative Supramolecular Polymers under Thermodynamic Control. Journal of the American Chemical Society, 2019, 141, 18278-18285.	13.7	52
24	Elucidation of the origin of chiral amplification in discrete molecular polyhedra. Nature Communications, 2018, 9, 488.	12.8	51
25	Self-Reproduction of Fatty Acid Vesicles: A Combined Experimental andÂSimulation Study. Biophysical Journal, 2010, 99, 1520-1528.	0.5	50
26	Photodynamic Control of the Chain Length in Supramolecular Polymers: Switching an Intercalator into a Chain Capper. Journal of the American Chemical Society, 2020, 142, 6295-6303.	13.7	47
27	Threshold Sensing through a Synthetic Enzymatic Reactionâ€“Diffusion Network. Angewandte Chemie - International Edition, 2014, 53, 8066-8069.	13.8	46
28	Counterion-Dependent Mechanisms of DNA Origami Nanostructure Stabilization Revealed by Atomistic Molecular Simulation. ACS Nano, 2019, 13, 10798-10809.	14.6	44
29	Vesicle Deformation by Draining: Geometrical and Topological Shape Changes. Journal of Physical Chemistry B, 2009, 113, 8731-8737.	2.6	41
30	Allosterically Controlled Threading of Polymers through Macrocyclic Dimers. Journal of the American Chemical Society, 2015, 137, 3915-3923.	13.7	40
31	Chain Growth by CO Insertion in the Fischerâ€“Tropsch Reaction. ChemCatChem, 2013, 5, 3384-3397.	3.7	37
32	Equilibrium Model for Supramolecular Copolymerizations. Journal of Physical Chemistry B, 2019, 123, 6627-6642.	2.6	36
33	Consequences of Cooperativity in Racemizing Supramolecular Systems. Angewandte Chemie - International Edition, 2012, 51, 6426-6431.	13.8	35
34	Fragmentation and Coagulation in Supramolecular (Co)polymerization Kinetics. ACS Central Science, 2016, 2, 232-241.	11.3	35
35	Coarse-Grained Transmembrane Proteins:â€‰ Hydrophobic Matching, Aggregation, and Their Effect on Fusion. Journal of Physical Chemistry B, 2006, 110, 13614-13623.	2.6	32
36	Conformational Analysis of Chiral Supramolecular Aggregates: Modeling the Subtle Difference between Hydrogen and Deuterium. Journal of the American Chemical Society, 2013, 135, 16497-16506.	13.7	31

#	Article	IF	Citations
37	Coarse Grained Molecular Dynamics Simulations of Transmembrane Protein-Lipid Systems. International Journal of Molecular Sciences, 2010, 11, 2393-2420.	4.1	25
38	Ultrasensitivity by Molecular Titration in Spatially Propagating Enzymatic Reactions. Biophysical Journal, 2013, 105, 1057-1066.	0.5	25
39	Detailed Approach to Investigate Thermodynamically Controlled Supramolecular Copolymerizations. Macromolecules, 2019, 52, 7430-7438.	4.8	25
40	Pathway Complexity in the Stacking of Imine-Linked Macrocycles Related to Two-Dimensional Covalent Organic Frameworks. Chemistry of Materials, 2019, 31, 7104-7111.	6.7	22
41	The CUMULUS Coarse Graining Method: Transferable Potentials for Water and Solutes. Journal of Physical Chemistry B, 2011, 115, 10001-10012.	2.6	20
42	Proteomic Analysis in Type 2 Diabetes Patients before and after a Very Low Calorie Diet Reveals Potential Disease State and Intervention Specific Biomarkers. PLoS ONE, 2014, 9, e112835.	2.5	19
43	Computer simulations of cellular group selection reveal mechanism for sustaining cooperation. Journal of Theoretical Biology, 2014, 357, 123-133.	1.7	17
44	Directional interactions in semiflexible single-chain polymer folding. Soft Matter, 2012, 8, 7610.	2.7	16
45	Evaporative self-assembly of single-chain, polymeric nanoparticles. Chemical Communications, 2013, 49, 3122.	4.1	16
46	Catalyst nano-particle size dependence of the Fischerâ€“Tropsch reaction. Faraday Discussions, 2013, 162, 267.	3.2	16
47	Molecular Simulation of Protein Encapsulation in Vesicle Formation. Journal of Physical Chemistry B, 2014, 118, 3346-3354.	2.6	16
48	On Protein Crowding and Bilayer Bulging in Spontaneous Vesicle Formation. Journal of Physical Chemistry B, 2012, 116, 12677-12683.	2.6	12
49	Mass-Balance Models for Scrutinizing Supramolecular (Co)polymerizations in Thermodynamic Equilibrium. Accounts of Chemical Research, 2019, 52, 3465-3474.	15.6	12
50	Density distribution for a dense hard-sphere gas in micro/nano-channels: Analytical and simulation results. Journal of Computational Physics, 2006, 219, 532-552.	3.8	11
51	Coarse-grained modelling of urea-adamantyl functionalised poly(propylene imine) dendrimers. Molecular Simulation, 2016, 42, 882-895.	2.0	11
52	Photoisomerization induced scission of rod-like micelles unravelled with multiscale modeling. Journal of Colloid and Interface Science, 2018, 510, 357-367.	9.4	11
53	Local Thomasâ€“Fermi approximation for modeling the electronic structure of planar devices. Physica B: Condensed Matter, 2003, 325, 149-156.	2.7	9
54	Designed Asymmetric Protein Assembly on a Symmetric Scaffold. Angewandte Chemie - International Edition, 2020, 59, 12113-12121.	13.8	8

#	Article	IF	Citations
55	Velocity Correlations and Accommodation Coefficients for Gas-Wall Interactions in Nanochannels. , 2008, , .		5
56	Methods for Multiscale Modeling of Membranes. Behavior Research Methods, 2012, 15, 139-170.	4.0	4
57	Multivalency in a Dendritic Hostâ€“Guest System. Macromolecules, 2019, 52, 2778-2788.	4.8	4
58	Laterally coupled jellium-like two-dimensional quantum dots. Journal of Physics Condensed Matter, 2003, 15, 6977-6984.	1.8	3
59	Fully local orbital-free calculation of electronic structure using pseudopotentials. Physica B: Condensed Matter, 2003, 339, 119-129.	2.7	2
60	A novel Method for Coarse Graining of Atomistic Simulations Using Boltzmann Inversion. Biophysical Journal, 2011, 100, 309a.	0.5	2
61	Designed Asymmetric Protein Assembly on a Symmetric Scaffold. Angewandte Chemie, 2020, 132, 12211-12219.	2.0	2
62	Local functional derivative of the total energy and the shell structure in atoms and molecules. Computational and Theoretical Chemistry, 2003, 638, 91-98.	1.5	1
63	Velocity Correlations Between Impinging and Reflecting Particles Using MD Simulations and Different Wall Models. , 2008, , .		1
64	Reflection of finite-width edge channels. Physical Review B, 1996, 54, 2806-2812.	3.2	0
65	New Derivation of a Particle Wall Boundary Condition in Molecular Dynamics. , 2007, , 767.		0
66	A Coarse Grained Molecular Dynamics Study of Self-Reproduction of Fatty Acid Vesicles. Biophysical Journal, 2010, 98, 272a.	0.5	0
67	Reproduction of Fatty Acid Vesicles. Biophysical Journal, 2010, 98, 272a.	0.5	0
68	Reproduction of Vesicles upon Fatty Acid Addition. Biophysical Journal, 2011, 100, 330a.	0.5	0
69	Protonation and the Matrix Effect of Oleate Vesicles, a Coarse Grained Molecular Dynamics Study. Biophysical Journal, 2012, 102, 397a.	0.5	0