Ahmed E Ismail

List of Publications by Year
in descending order

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Version: 2024-02-01

42 papers	2,198 citations	304743 22 h-index	276875 41 g-index
44 all docs	44 docs citations	44 times ranked	3108 citing authors

#	Article	IF	Citations
1	On the Applicability of Force Fields To Study the Aggregation of Amyloidogenic Peptides Using Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 6063-6075.	5.3	68
2	Accelerating molecular dynamics codes by performance and accuracy modeling. Journal of Computational Science, 2018, 27, 77-90.	2.9	2
3	Industrial Applications of Enzymes: Recent Advances, Techniques, and Outlooks. Catalysts, 2018, 8, 238.	3.5	509
4	Î± to Î² mechano-conversion and amorphization in native cellulose simulated by crystal bending. Cellulose, 2018, 25, 4345-4355.	4.9	14
5	Translational Entropy and Dispersion Energy Jointly Drive the Adsorption of Urea to Cellulose. Journal of Physical Chemistry B, 2017, 121, 2244-2251.	2.6	28
6	Theory of wavelet-based coarse-graining hierarchies for molecular dynamics. Physical Review E, 2017, 96, 013301.	2.1	1
7	Multiresolution Modeling of Semidilute Polymer Solutions: Coarse-Graining Using Wavelet-Accelerated Monte Carlo. Computation, 2017, 5, 44.	2.0	0
8	LAMMPSâ€™ PPPM Long-Range Solver for the Second Generation Xeon Phi. Lecture Notes in Computer Science, 2017, , 61-78.	1.3	6
9	Requirements for the Formation and Shape of Microscopic Precursors in Droplet Spreading. Langmuir, 2016, 32, 4472-4478.	3.5	10
10	Mechanisms of hydrogen bond formation between ionic liquids and cellulose and the influence of water content. Physical Chemistry Chemical Physics, 2015, 17, 5767-5775.	2.8	91
11	Oligomer Formation of Toxic and Functional Amyloid Peptides Studied with Atomistic Simulations. Journal of Physical Chemistry B, 2015, 119, 9696-9705.	2.6	29
12	Smoothing of contact lines in spreading droplets by trisiloxane surfactants and its relevance for superspreading. Soft Matter, 2015, 11, 4527-4539.	2.7	13
13	Automated Discovery of Reaction Pathways, Rate Constants, and Transition States Using Reactive Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2517-2524.	5.3	155
14	Diffusion Wavelet Decomposition for Coarse-Graining of Polymer Chains. Materials Research Society Symposia Proceedings, 2015, 1753, 24.	0.1	0
15	Effect of Water Content in N-Methylmorpholine N-Oxide/Cellulose Solutions on Thermodynamics, Structure, and Hydrogen Bonding. Journal of Physical Chemistry B, 2015, 119, 15014-15022.	2.6	38
16	Multilevel summation for dispersion: A linear-time algorithm for râ€‰â^'6 potentials. Journal of Chemical Physics, 2014, 140, 024105.	3.0	19
17	Coating thickness and coverage effects on the forces between silica nanoparticles in water. Journal of Chemical Physics, 2014, 140, 194904.	3.0	28
18	Atomistic Potentials for Trisiloxane, Alkyl Ethoxylate, and Perfluoroalkane-Based Surfactants with TIP4P/2005 and Application to Simulations at the Airâ€“Water Interface. Journal of Physical Chemistry B, 2014, 118, 9284-9297.	2.6	9

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19	The Role of the Cation in the Solvation of Cellulose by Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 1621-1629.	2.6	84
20	Multiscale treatment of mechanical contact problems involving thin polymeric layers. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 045012.	2.0	3
21	Observed Mechanism for the Breakup of Small Bundles of Cellulose Iβ and Iα in Ionic Liquids from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 3469-3479.	2.6	95
22	Effects of Water Concentration on the Structural and Diffusion Properties of Imidazolium-Based Ionic Liquidâ€“Water Mixtures. Journal of Physical Chemistry B, 2013, 117, 1378-1388.	2.6	111
23	Reconsidering Dispersion Potentials: Reduced Cutoffs in Mesh-Based Ewald Solvers Can Be Faster Than Truncation. Journal of Chemical Theory and Computation, 2013, 9, 5412-5420.	5.3	47
24	Development and application of a particle-particle particle-mesh Ewald method for dispersion interactions. Journal of Chemical Physics, 2012, 137, 174107.	3.0	112
25	Definition and Computation of Intermolecular Contact in Liquids Using Additively Weighted Voronoi Tessellation. Journal of Physical Chemistry A, 2012, 116, 4657-4666.	2.5	12
26	Fully Atomistic Simulations of the Response of Silica Nanoparticle Coatings to Alkane Solvents. Langmuir, 2012, 28, 17443-17449.	3.5	33
27	The Effects of Chloride Binding on the Behavior of Cellulose-Derived Solutes in the Ionic Liquid 1-Butyl-3-methylimidazolium Chloride. Journal of Physical Chemistry B, 2012, 116, 9732-9743.	2.6	10
28	Diffusion of small penetrant molecules in polybutadienes. Molecular Physics, 2011, 109, 2025-2033.	1.7	9
29	Solubility of Fe2(OH)3Cl (pure-iron end-member of hibbingite) in NaCl and Na2SO4 brines. Chemical Geology, 2011, 280, 26-32.	3.3	18
30	Electronâ€“ion coupling effects on simulations of radiation damage in pyrochlore waste forms. Journal of Physics Condensed Matter, 2010, 22, 225405.	1.8	17
31	Interfacial Structure and Dynamics of Siloxane Systems: PDMSâ^'Vapor and PDMSâ^'Water. Macromolecules, 2009, 42, 3186-3194.	4.8	74
32	Forces between functionalized silica nanoparticles in solution. Physical Review E, 2009, 79, 050501.	2.1	53
33	Surface tension of normal and branched alkanes. Molecular Physics, 2007, 105, 3155-3163.	1.7	45
34	Application of Ewald summations to long-range dispersion forces. Journal of Chemical Physics, 2007, 127, 144711.	3.0	141
35	Structure and Dynamics of Water near the Interface with Oligo(ethylene oxide) Self-Assembled Monolayers. Langmuir, 2007, 23, 8508-8514.	3.5	35
36	Capillary waves at the liquid-vapor interface and the surface tension of water. Journal of Chemical Physics, 2006, 125, 014702.	3.0	155

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37	Using wavelet transforms for multiresolution materials modeling. Computers and Chemical Engineering, 2005, 29, 689-700.	3.8	8
38	Wavelet-accelerated Monte Carlo sampling of polymer chains. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 897-910.	2.1	2
39	Topological coarse graining of polymer chains using wavelet-accelerated Monte Carlo. II. Self-avoiding chains. Journal of Chemical Physics, 2005, 122, 234902.	3.0	6
40	Topological coarse graining of polymer chains using wavelet-accelerated Monte Carlo. I. Freely jointed chains. Journal of Chemical Physics, 2005, 122, 234901.	3.0	8
41	Multiresolution analysis in statistical mechanics. II. The wavelet transform as a basis for Monte Carlo simulations on lattices. Journal of Chemical Physics, 2003, 118, 4424-4431.	3.0	45
42	Multiresolution analysis in statistical mechanics. I. Using wavelets to calculate thermodynamic properties. Journal of Chemical Physics, 2003, 118, 4414-4423.	3.0	52