Ahmed E Ismail

List of Publications by Year
in descending order

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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	Industrial Applications of Enzymes: Recent Advances, Techniques, and Outlooks. Catalysts, 2018, 8, 238.	3.5	509
2	Capillary waves at the liquid-vapor interface and the surface tension of water. Journal of Chemical Physics, 2006, 125, 014702.	3.0	155
3	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
4	Application of Ewald summations to long-range dispersion forces. Journal of Chemical Physics, 2007, 127, 144711.	3.0	141
5	Development and application of a particle-particle particle-mesh Ewald method for dispersion interactions. Journal of Chemical Physics, 2012, 137, 174107.	3.0	112
6	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
7	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
8	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
9	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
10	Interfacial Structure and Dynamics of Siloxane Systems: PDMSâ^'Vapor and PDMSâ^'Water. Macromolecules, 2009, 42, 3186-3194.	4.8	74
11	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
12	Forces between functionalized silica nanoparticles in solution. Physical Review E, 2009, 79, 050501.	2.1	53
13	Multiresolution analysis in statistical mechanics. I. Using wavelets to calculate thermodynamic properties. Journal of Chemical Physics, 2003, 118, 4414-4423.	3.0	52
14	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
15	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
16	Surface tension of normal and branched alkanes. Molecular Physics, 2007, 105, 3155-3163.	1.7	45
17	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
18	Structure and Dynamics of Water near the Interface with Oligo(ethylene oxide) Self-Assembled Monolayers. Langmuir, 2007, 23, 8508-8514.	3.5	35

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19	Fully Atomistic Simulations of the Response of Silica Nanoparticle Coatings to Alkane Solvents. Langmuir, 2012, 28, 17443-17449.	3.5	33
20	Oligomer Formation of Toxic and Functional Amyloid Peptides Studied with Atomistic Simulations. Journal of Physical Chemistry B, 2015, 119, 9696-9705.	2.6	29
21	Coating thickness and coverage effects on the forces between silica nanoparticles in water. Journal of Chemical Physics, 2014, 140, 194904.	3.0	28
22	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
23	Multilevel summation for dispersion: A linear-time algorithm for râ€‰â^'6 potentials. Journal of Chemical Physics, 2014, 140, 024105.	3.0	19
24	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
25	Electronâ€“ion coupling effects on simulations of radiation damage in pyrochlore waste forms. Journal of Physics Condensed Matter, 2010, 22, 225405.	1.8	17
26	Îİ± to Îİ² mechano-conversion and amorphization in native cellulose simulated by crystal bending. Cellulose, 2018, 25, 4345-4355.	4.9	14
27	Smoothing of contact lines in spreading droplets by trisiloxane surfactants and its relevance for superspreading. Soft Matter, 2015, 11, 4527-4539.	2.7	13
28	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
29	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
30	Requirements for the Formation and Shape of Microscopic Precursors in Droplet Spreading. Langmuir, 2016, 32, 4472-4478.	3.5	10
31	Diffusion of small penetrant molecules in polybutadienes. Molecular Physics, 2011, 109, 2025-2033.	1.7	9
32	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
33	Using wavelet transforms for multiresolution materials modeling. Computers and Chemical Engineering, 2005, 29, 689-700.	3.8	8
34	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
35	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
36	LAMMPSâ€™ PPPM Long-Range Solver for the Second Generation Xeon Phi. Lecture Notes in Computer Science, 2017, , 61-78.	1.3	6

#	Article	IF	Citations
37	Multiscale treatment of mechanical contact problems involving thin polymeric layers. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 045012.	2.0	3
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	Accelerating molecular dynamics codes by performance and accuracy modeling. Journal of Computational Science, 2018, 27, 77-90.	2.9	2
40	Theory of wavelet-based coarse-graining hierarchies for molecular dynamics. Physical Review E, 2017, 96, 013301.	2.1	1
41	Diffusion Wavelet Decomposition for Coarse-Graining of Polymer Chains. Materials Research Society Symposia Proceedings, 2015, 1753, 24.	0.1	0
42	Multiresolution Modeling of Semidilute Polymer Solutions: Coarse-Graining Using Wavelet-Accelerated Monte Carlo. Computation, 2017, 5, 44.	2.0	0