Alan E Mark

List of Publications by Citations

223 papers	35,808 citations	72 h-index	188 g-index
229 ext. papers	40,010 ext. citations	5.4 avg, IF	7.24 L-index

#	Paper	IF	Citations
223	GROMACS: fast, flexible, and free. *Journal of Computational Chemistry*, **2005**, 26, 1701-18	3.5	10273
222	A biomolecular force field based on the free enthalpy of hydration and solvation: the GROMOS force-field parameter sets 53A5 and 53A6. *Journal of Computational Chemistry*, **2004**, 25, 1656-76	3.5	2844
221	Coarse Grained Model for Semiquantitative Lipid Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 750-760	3.4	1767
220	Definition and testing of the GROMOS force-field versions 54A7 and 54B7. *European Biophysics Journal*, **2011**, 40, 843-56	1.9	1326
219	Peptide Folding: When Simulation Meets Experiment. *Angewandte Chemie - International Edition*, **1999**, 38, 236-240	16.4	1258
218	The GROMOS Biomolecular Simulation Program Package. *Journal of Physical Chemistry A*, **1999**, 103, 3596-3607	2.8	1220
217	An Automated Force Field Topology Builder (ATB) and Repository: Version 1.0. *Journal of Chemical Theory and Computation*, **2011**, 7, 4026-37	6.4	1030
216	Avoiding singularities and numerical instabilities in free energy calculations based on molecular simulations. *Chemical Physics Letters*, **1994**, 222, 529-539	2.5	819
215	Mechanism by which 2,2,2-trifluoroethanol/water mixtures stabilize secondary-structure formation in peptides: a molecular dynamics study. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 12179-84	11.5	406
214	Antimicrobial peptides in action. *Journal of the American Chemical Society*, **2006**, 128, 12156-61	16.4	372
213	Toroidal pores formed by antimicrobial peptides show significant disorder. *Biochimica Et Biophysica Acta - Biomembranes*, **2008**, 1778, 2308-17	3.8	364
212	Simulation of pore formation in lipid bilayers by mechanical stress and electric fields. *Journal of the American Chemical Society*, **2003**, 125, 6382-3	16.4	363
211	Reversible peptide folding in solution by molecular dynamics simulation. *Journal of Molecular Biology*, **1998**, 280, 925-32	6.5	340
210	Parametrization of aliphatic CHn united atoms of GROMOS96 force field **1998**, 19, 535-547		335
209	Testing and validation of the Automated Topology Builder (ATB) version 2.0: prediction of hydration free enthalpies. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 221-33	4.2	334
208	Fluctuation and cross-correlation analysis of protein motions observed in nanosecond molecular dynamics simulations. *Journal of Molecular Biology*, **1995**, 252, 492-503	6.5	332
207	Folding-unfolding thermodynamics of a beta-heptapeptide from equilibrium simulations. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 269-80	4.2	330

206	Decomposition of the free energy of a system in terms of specific interactions. Implications for theoretical and experimental studies. *Journal of Molecular Biology*, **1994**, 240, 167-76	6.5	289
205	The mechanism of vesicle fusion as revealed by molecular dynamics simulations. *Journal of the American Chemical Society*, **2003**, 125, 11144-5	16.4	278
204	Mechanism of activation of protein kinase JAK2 by the growth hormone receptor. *Science*, **2014**, 344, 1249783	33.3	269
203	Molecular dynamics simulation of the formation, structure, and dynamics of small phospholipid vesicles. *Journal of the American Chemical Society*, **2003**, 125, 15233-42	16.4	263
202	A new force field for simulating phosphatidylcholine bilayers. *Journal of Computational Chemistry*, **2010**, 31, 1117-25	3.5	261
201	Simulation of gel phase formation and melting in lipid bilayers using a coarse grained model. *Chemistry and Physics of Lipids*, **2005**, 135, 223-44	3.7	261
200	Molecular dynamics simulations of hydrophilic pores in lipid bilayers. *Biophysical Journal*, **2004**, 86, 2156-64	3.9	248
199	Molecular Dynamics Simulation of the Kinetics of Spontaneous Micelle Formation. *Journal of Physical Chemistry B*, **2000**, 104, 12165-12173	3.4	248
198	Photoactivation of the photoactive yellow protein: why photon absorption triggers a trans-to-cis Isomerization of the chromophore in the protein. *Journal of the American Chemical Society*, **2004**, 126, 4228-33	16.4	246
197	Effect of Undulations on Surface Tension in Simulated Bilayers. *Journal of Physical Chemistry B*, **2001**, 105, 6122-6127	3.4	237
196	On the Validation of Molecular Dynamics Simulations of Saturated and cis-Monounsaturated Phosphatidylcholine Lipid Bilayers: A Comparison with Experiment. *Journal of Chemical Theory and Computation*, **2010**, 6, 325-36	6.4	232
195	Basic ingredients of free energy calculations: a review. *Journal of Computational Chemistry*, **2010**, 31, 1569-82	3.5	225
194	Simulation of the spontaneous aggregation of phospholipids into bilayers. *Journal of the American Chemical Society*, **2001**, 123, 8638-9	16.4	223
193	Monolayer ice. *Physical Review Letters*, **2003**, 91, 025502	7.4	195
192	Automated Topology Builder Version 3.0: Prediction of Solvation Free Enthalpies in Water and Hexane. *Journal of Chemical Theory and Computation*, **2018**, 14, 5834-5845	6.4	174
191	Solvent-dependent conformation and hydrogen-bonding capacity of cyclosporin A: evidence from partition coefficients and molecular dynamics simulations. *Journal of Medicinal Chemistry*, **1993**, 36, 3757-64	8.3	169
190	Molecular view of hexagonal phase formation in phospholipid membranes. *Biophysical Journal*, **2004**, 87, 3894-900	2.9	167
189	Dielectric properties of trypsin inhibitor and lysozyme calculated from molecular dynamics simulations. *The Journal of Physical Chemistry*, **1993**, 97, 2009-2014		167

188	Absolute entropies from molecular dynamics simulation trajectories. *Journal of Chemical Physics*, **2000**, 113, 7809-7817	3.9	158
187	Calculation of the free energy of solvation for neutral analogs of amino acid side chains. *Journal of Computational Chemistry*, **2002**, 23, 548-53	3.5	157
186	Refinement of homology-based protein structures by molecular dynamics simulation techniques. *Protein Science*, **2004**, 13, 211-20	6.3	154
185	Molecular simulation as an aid to experimentalists. *Current Opinion in Structural Biology*, **2008**, 18, 149-53	8.1	150
184	Molecular dynamics simulation of the spontaneous formation of a small DPPC vesicle in water in atomistic detail. *Journal of the American Chemical Society*, **2004**, 126, 4488-9	16.4	150
183	Convergence Properties of Free Energy Calculations: .alpha.-Cyclodextrin Complexes as a Case Study. *Journal of the American Chemical Society*, **1994**, 116, 6293-6302	16.4	150
182	Molecular structure of the lecithin ripple phase. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 5392-6	11.5	146
181	Estimating the Relative Free Energy of Different Molecular States with Respect to a Single Reference State. *The Journal of Physical Chemistry*, **1996**, 100, 9485-9494		146
180	Alternative mechanisms for the interaction of the cell-penetrating peptides penetratin and the TAT peptide with lipid bilayers. *Biophysical Journal*, **2009**, 97, 40-9	2.9	143
179	Simulation of the thermal denaturation of hen egg white lysozyme: trapping the molten globule state. *Biochemistry*, **1992**, 31, 7745-8	3.2	141
178	Validation of molecular dynamics simulation. *Journal of Chemical Physics*, **1998**, 108, 6109-6116	3.9	139
177	Charge group partitioning in biomolecular simulation. *Journal of Computational Biology*, **2013**, 20, 188-98	1.7	120
176	The Role of histidine residues in low-pH-mediated viral membrane fusion. *Structure*, **2006**, 14, 1481-7	5.2	120
175	The effect of force-field parameters on properties of liquids: Parametrization of a simple three-site model for methanol. *Journal of Chemical Physics*, **2000**, 112, 10450-10459	3.9	120
174	Comparison of MD simulations and NMR experiments for hen lysozyme. Analysis of local fluctuations, cooperative motions, and global changes. *Biochemistry*, **1995**, 34, 10918-31	3.2	120
173	Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. *Journal of Molecular Biology*, **2001**, 309, 299-313	6.5	119
172	Bilayer ice and alternate liquid phases of confined water. *Journal of Chemical Physics*, **2003**, 119, 1694-1700	3.9	114
171	Dynamic Conformations of Flavin Adenine Dinucleotide: Simulated Molecular Dynamics of the Flavin Cofactor Related to the Time-Resolved Fluorescence Characteristics. *Journal of Physical Chemistry B*, **2002**, 106, 8858-8869	3.4	113

170	Developments in Glycopeptide Antibiotics. *ACS Infectious Diseases*, **2018**, 4, 715-735	5.5	112
169	Convergence and sampling efficiency in replica exchange simulations of peptide folding in explicit solvent. *Journal of Chemical Physics*, **2007**, 126, 014903	3.9	105
168	On the interpretation of biochemical data by molecular dynamics computer simulation. *FEBS Journal*, **1992**, 204, 947-61		105
167	The Binary Mixing Behavior of Phospholipids in a Bilayer: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2004**, 108, 2454-2463	3.4	104
166	Electrofreezing of confined water. *Journal of Chemical Physics*, **2004**, 120, 7123-30	3.9	99
165	A New 2,2,2-Trifluoroethanol Model for Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2000**, 104, 12347-12354	3.4	99
164	Understanding binding affinity: a combined isothermal titration calorimetry/molecular dynamics study of the binding of a series of hydrophobically modified benzamidinium chloride inhibitors to trypsin. *Journal of the American Chemical Society*, **2003**, 125, 10570-9	16.4	90
163	On the characterization of host-guest complexes: surface tension, calorimetry, and molecular dynamics of cyclodextrins with a non-ionic surfactant. *Journal of Physical Chemistry B*, **2007**, 111, 4383-92	3.4	89
162	Computational approaches to study protein unfolding: hen egg white lysozyme as a case study. *Proteins: Structure, Function and Bioinformatics*, **1995**, 21, 196-213	4.2	89
161	Computation of Free Energy. *Helvetica Chimica Acta*, **2002**, 85, 3113-3129	2	85
160	Entropy calculations on a reversibly folding peptide: changes in solute free energy cannot explain folding behavior. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 45-56	4.2	85
159	The effect of motional averaging on the calculation of NMR-derived structural properties **1999**, 36, 542-555		83
158	Does isoprene protect plant membranes from thermal shock? A molecular dynamics study. *Biochimica Et Biophysica Acta - Biomembranes*, **2007**, 1768, 198-206	3.8	81
157	Molecular dynamics simulations of mixed micelles modeling human bile. *Biochemistry*, **2002**, 41, 5375-82	3.2	81
156	A ring to rule them all: the effect of cyclopropane Fatty acids on the fluidity of lipid bilayers. *Journal of Physical Chemistry B*, **2015**, 119, 5487-95	3.4	80
155	Ion transport across transmembrane pores. *Biophysical Journal*, **2007**, 92, 4209-15	2.9	80
154	A dynamic pharmacophore drives the interaction between Psalmotoxin-1 and the putative drug target acid-sensing ion channel 1a. *Molecular Pharmacology*, **2011**, 80, 796-808	4.3	78
153	Validation of Molecular Simulation: An Overview of Issues. *Angewandte Chemie - International Edition*, **2018**, 57, 884-902	16.4	74

152	Weak, strong, and coherent regimes of Frölich condensation and their applications to terahertz medicine and quantum consciousness. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 4219-24	11.5	74
151	The CC domain structure from the wheat stem rust resistance protein Sr33 challenges paradigms for dimerization in plant NLR proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12856-12861	11.5	72
150	Can the stability of protein mutants be predicted by free energy calculations?. *Protein Engineering, Design and Selection*, **1993**, 6, 289-95	1.9	72
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148	Simulation of MscL gating in a bilayer under stress. *Biophysical Journal*, **2003**, 84, 2331-7	2.9	67
147	Lipid Bilayers: The Effect of Force Field on Ordering and Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 4807-17	6.4	66
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143	Signal transduction in the photoactive yellow protein. I. Photon absorption and the isomerization of the chromophore. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 202-11	4.2	61
142	The Cys3-Cys4 loop of the hydrophobin EAS is not required for rodlet formation and surface activity. *Journal of Molecular Biology*, **2008**, 382, 708-20	6.5	60
141	Application of mean field boundary potentials in simulations of lipid vesicles. *Journal of Physical Chemistry B*, **2008**, 112, 7438-47	3.4	57
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139	Estimating relative free energies from a single ensemble: Hydration free energies. *Journal of Computational Chemistry*, **1999**, 20, 1604-1617	3.5	55
138	Factors that affect the degree of twist in beta-sheet structures: a molecular dynamics simulation study of a cross-beta filament of the GNNQQNY peptide. *Journal of Physical Chemistry B*, **2009**, 113, 1728-37	3.4	54
137	Peptide Folding: When Simulation Meets Experiment **1999**, 38, 236		54
136	Molecular dynamics simulations of the interactions of DMSO with DPPC and DOPC phospholipid membranes. *Journal of Physical Chemistry B*, **2012**, 116, 11911-23	3.4	53
135	Interaction of Tarantula Venom Peptide ProTx-II with Lipid Membranes Is a Prerequisite for Its Inhibition of Human Voltage-gated Sodium Channel NaV1.7. *Journal of Biological Chemistry*, **2016**, 291, 17049-65	5.4	52

134	Validating lipid force fields against experimental data: Progress, challenges and perspectives. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1556-65	3.8	51
133	Histidine protonation and the activation of viral fusion proteins. *Biochemical Society Transactions*, **2008**, 36, 43-5	5.1	51
132	Peptidfaltung: Wenn die Simulation das Experiment erreicht. *Angewandte Chemie*, **1999**, 111, 249-253	3.6	51
131	Effect of methyl-branched fatty acids on the structure of lipid bilayers. *Journal of Physical Chemistry B*, **2014**, 118, 13838-48	3.4	49
130	Penrose-Hameroff orchestrated objective-reduction proposal for human consciousness is not biologically feasible. *Physical Review E*, **2009**, 80, 021912	2.4	48
129	Simulation studies of pore and domain formation in a phospholipid monolayer. *Journal of Chemical Physics*, **2005**, 122, 024704	3.9	48
128	Computer simulation of protein motion. *Computer Physics Communications*, **1995**, 91, 305-319	4.2	48
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125	Calculation of the redox potential of the protein azurin and some mutants. *ChemBioChem*, **2005**, 6, 738-46	3.8	46
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123	Folding and stability of the three-stranded beta-sheet peptide Betanova: insights from molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 380-92	4.2	45
122	Relative stability of protein structures determined by X-ray crystallography or NMR spectroscopy: a molecular dynamics simulation study. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 111-20	4.2	44
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113	Prediction of the activity and stability effects of site-directed mutagenesis on a protein core. *Journal of Molecular Biology*, **1992**, 227, 389-95	6.5	39
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111	An approximate but efficient method to calculate free energy trends by computer simulation: application to dihydrofolate reductase-inhibitor complexes. *Journal of Computer-Aided Molecular Design*, **1993**, 7, 305-23	4.2	38
110	Real Cost of Speed: The Effect of a Time-Saving Multiple-Time-Stepping Algorithm on the Accuracy of Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 2367-2372	6.4	36
109	Comparison of enveloping distribution sampling and thermodynamic integration to calculate binding free energies of phenylethanolamine N-methyltransferase inhibitors. *Journal of Chemical Physics*, **2011**, 135, 024105	3.9	36
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105	The structure of a two-disulfide intermediate assists in elucidating the oxidative folding pathway of a cyclic cystine knot protein. *Structure*, **2008**, 16, 842-51	5.2	34
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102	Elucidating the Spatial Arrangement of Emitter Molecules in Organic Light-Emitting Diode Films. *Angewandte Chemie - International Edition*, **2017**, 56, 8402-8406	16.4	33
101	Peptide folding simulations: no solvent required?. *Computer Physics Communications*, **1999**, 123, 97-102	4.2	32
100	The Molecular Origin of Anisotropic Emission in an Organic Light-Emitting Diode. *Nano Letters*, **2017**, 17, 6464-6468	11.5	30
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97	The effect of environment on the recognition and binding of vancomycin to native and resistant forms of lipid II. *Biophysical Journal*, **2011**, 101, 2684-92	2.9	28
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95	The effect of box shape on the dynamic properties of proteins simulated under periodic boundary conditions. *Journal of Computational Chemistry*, **2006**, 27, 316-25	3.5	28
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92	Effect of high pressure on fully hydrated DPPC and POPC bilayers. *Journal of Physical Chemistry B*, **2011**, 115, 1038-44	3.4	26
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90	On using time-averaging restraints in molecular dynamics simulation. *Journal of Biomolecular NMR*, **1998**, 12, 501-8	3	25
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84	A molecular dynamics study of the formation, stability, and oligomerization state of two designed coiled coils: possibilities and limitations. *Biophysical Journal*, **2005**, 89, 3701-13	2.9	23
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79	Missing fragments: detecting cooperative binding in fragment-based drug design. *ACS Medicinal Chemistry Letters*, **2012**, 3, 322-6	4.3	21
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64	Optimization of Empirical Force Fields by Parameter Space Mapping: A Single-Step Perturbation Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 6201-6212	6.4	16
63	Molecular dynamics unlocks atomic level self-assembly of the exopolysaccharide matrix of water-treatment granular biofilms. *Biomacromolecules*, **2012**, 13, 1965-72	6.9	16

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57	GROMOS Force Field		14
56	Automated partial atomic charge assignment for drug-like molecules: a fast knapsack approach. *Algorithms for Molecular Biology*, **2019**, 14, 1	1.8	13
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