Andrij Baumketner

List of Publications by Year
in descending order

60 papers	2,264 citations	346980 22 h-index	242451 47 g-index
60 all docs	60 docs citations	60 times ranked	2516 citing authors

#	Article	IF	Citations
1	Liquidâ€“gas critical point of a two-dimensional system of hard ellipses with attractive wells. Journal of Chemical Physics, 2022, 156, 034102.	1.2	2
2	Kagome lattice made by impenetrable ellipses with attractive walls. Soft Matter, 2022, 18, 3801-3814.	1.2	1
3	On the Mechanism of Alkylammonium Ligands Binding to the Surface of CsPbBr₃ Nanocrystals. Chemistry of Materials, 2021, 33, 5962-5973.	3.2	39
4	Attraction between Like-Charged Macroions Mediated by Specific Counterion Configurations. Journal of Physical Chemistry B, 2019, 123, 9971-9983.	1.2	4
5	Cluster Crystals Stabilized by Hydrophobic and Electrostatic Interactions. Journal of Physical Chemistry B, 2018, 122, 2669-2682.	1.2	5
6	Clusters of lysozyme in aqueous solutions. Physical Review E, 2018, 98, .	0.8	6
7	Softness and non-spherical shape define the phase behavior and the structural properties of lysozyme in aqueous solutions. Journal of Chemical Physics, 2016, 144, 015103.	1.2	5
8	Equilibrium clusters in suspensions of colloids interacting via potentials with a local minimum. Condensed Matter Physics, 2016, 19, 13605.	0.3	8
9	Electric Field as a Disaggregating Agent for Amyloid Fibrils. Journal of Physical Chemistry B, 2014, 118, 14578-14589.	1.2	26
10	Reduced atomic pair-interaction design (RAPID) model for simulations of proteins. Journal of Chemical Physics, 2013, 138, 064102.	1.2	8
11	Generalized image charge solvation model for electrostatic interactions in molecular dynamics simulations of aqueous solutions. Journal of Computational Physics, 2013, 245, 84-106.	1.9	8
12	ICSM: An order method for calculating electrostatic interactions added to TINKER. Computer Physics Communications, 2013, 184, 19-26.	3.0	4
13	Effect of the Reaction Field on Molecular Forces and Torques Revealed by an Image-Charge Solvation Model. Communications in Computational Physics, 2013, 13, 129-149.	0.7	0
14	The mechanism of the converter domain rotation in the recovery stroke of myosin motor protein. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2701-2710.	1.5	16
15	Interactions between relay helix and Src homology 1 (SH1) domain helix drive the converter domain rotation during the recovery stroke of myosin II. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1569-1581.	1.5	5
16	Optimized Image Charges for Reaction Field Calculations. Biophysical Journal, 2011, 100, 157a.	0.2	0
17	Effect of atom- and group-based truncations on biomolecules simulated with reaction-field electrostatics. Journal of Molecular Modeling, 2011, 17, 2883-2893.	0.8	16
18	Early stages of the recovery stroke in myosin II studied by molecular dynamics simulations. Protein Science, 2011, 20, 2013-2022.	3.1	12

#	Article	IF	Citations
19	Ionic solvation studied by image-charge reaction field method. Journal of Chemical Physics, 2011, 134, 044105.	1.2	23
20	Testing a Hybrid Solvation Model with a Transition Layer Via Molecular Dynamics Simulation. Biophysical Journal, 2010, 98, 575a.	0.2	0
21	An image-based reaction field method for electrostatic interactions in molecular dynamics simulations of aqueous solutions. Journal of Chemical Physics, 2009, 131, 154103.	1.2	38
22	Removing systematic errors in interionic potentials of mean force computed in molecular simulations using reaction-field-based electrostatics. Journal of Chemical Physics, 2009, 130, 104106.	1.2	27
23	Amyloid Î²-Protein: Experiment and Theory on the 21â^'30 Fragment. Journal of Physical Chemistry B, 2009, 113, 6041-6046.	1.2	50
24	Microscopic Factors that Control Î²-Sheet Registry in Amyloid Fibrils Formed by Fragment 11â€“25 of Amyloid Î² Peptide: Insights from Computer Simulations. Journal of Molecular Biology, 2009, 389, 921-937.	2.0	14
25	A new FFT-based algorithm to compute Born radii in the generalized Born theory of biomolecule solvation. Journal of Computational Physics, 2008, 227, 10162-10177.	1.9	12
26	Effects of Familial Alzheimerâ€™s Disease Mutations on the Folding Nucleation of the Amyloid Î²-Protein. Journal of Molecular Biology, 2008, 381, 221-228.	2.0	96
27	Role of the familial Dutch mutation E22Q in the folding and aggregation of the 15â€“28 fragment of the Alzheimer amyloid-Î² protein. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6027-6032.	3.3	78
28	Stability of a protein tethered to a surface. Journal of Chemical Physics, 2007, 126, 095101.	1.2	38
29	The Structure of the Alzheimer Amyloid Î² 10-35 Peptide Probed through Replica-Exchange Molecular Dynamics Simulations in Explicit Solvent. Journal of Molecular Biology, 2007, 366, 275-285.	2.0	132
30	Elucidating Amyloid Î²-Protein Folding and Assembly:â€‰ A Multidisciplinary Approach. Accounts of Chemical Research, 2006, 39, 635-645.	7.6	203
31	Folding Landscapes of the Alzheimer Amyloid-Î²(12-28) Peptide. Journal of Molecular Biology, 2006, 362, 567-579.	2.0	74
32	Simulations of Protein Folding. Reviews in Computational Chemistry, 2006, , 169-228.	1.5	3
33	Amyloid beta-protein monomer structure: A computational and experimental study. Protein Science, 2006, 15, 420-428.	3.1	236
34	Structure of the 21-30 fragment of amyloid Î²-protein. Protein Science, 2006, 15, 1239-1247.	3.1	140
35	The Thermodynamics of Folding of a Î² Hairpin Peptide Probed Through Replica Exchange Molecular Dynamics Simulations. Theoretical Chemistry Accounts, 2006, 116, 262-273.	0.5	14
36	Effects of surface tethering on protein folding mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 8396-8401.	3.3	102

#	Article	IF	Citations
37	Aggregation of polyalanine in a hydrophobic environment. Journal of Chemical Physics, 2006, 124, 134904.	1.2	26
38	Free Energy Landscapes for Amyloidogenic Tetrapeptides Dimerization. Biophysical Journal, 2005, 89, 1493-1503.	0.2	55
39	Amyloid Î²-Protein:Â Monomer Structure and Early Aggregation States of AÎ²42 and Its Pro19Alloform. Journal of the American Chemical Society, 2005, 127, 2075-2084.	6.6	321
40	The Influence of Different Treatments of Electrostatic Interactions on the Thermodynamics of Folding of Peptides. Journal of Physical Chemistry B, 2005, 109, 21322-21328.	1.2	33
41	Improved theoretical description of protein folding kinetics from rotations in the phase space of relevant order parameters. Journal of Chemical Physics, 2004, 121, 1114-1120.	1.2	7
42	Viscoelastic model for the dynamic structure factors of binary systems. Physical Review E, 2004, 70, 041201.	0.8	21
43	Accelerated folding in the weak hydrophobic environment of a chaperonin cavity: Creation of an alternate fast folding pathway. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 13192-13197.	3.3	105
44	Effects of Confinement in Chaperonin Assisted Protein Folding: Rate Enhancement by Decreasing the Roughness of the Folding Energy Landscape. Journal of Molecular Biology, 2003, 332, 701-713.	2.0	111
45	Kinetics of the coil-to-helix transition on a rough energy landscape. Physical Review E, 2003, 68, 051901.	0.8	12
46	Glass transition in an off-lattice protein model studied by molecular dynamics simulations. Physical Review E, 2003, 67, 011912.	0.8	14
47	Molecular Dynamics Study of Protein Folding: Potentials and Mechanisms. AIP Conference Proceedings, 2003, , .	0.3	0
48	Diffusive dynamics of protein folding studied by molecular dynamics simulations of an off-lattice model. Physical Review E, 2002, 66, 011905.	0.8	16
49	Influence of the Hydrodynamic Interaction on Kinetics and Thermodynamics of Minimal Protein Models. Journal of the Physical Society of Japan, 2002, 71, 3069-3079.	0.7	9
50	Structural organization of a chain molecule with specific charge distribution: A molecular dynamics study. Molecular Simulation, 2002, 28, 359-375.	0.9	1
51	Stochastic tunneling minimization by molecular dynamics: an application to heteropolymer models. Physica A: Statistical Mechanics and Its Applications, 2002, 310, 139-150.	1.2	4
52	Running Multicanonical Simulations on Deformed Energy Surface: Application to a Model Protein. Journal of the Physical Society of Japan, 2002, 71, 1001-1002.	0.7	2
53	Finite-size dependence of the bridge function extracted from molecular dynamics simulations. Physical Review E, 2001, 63, 061201.	0.8	17
54	A Comparative Study of the Diffusion Processes in Liquid Binary Alloys with a Tendency to Aggregation and Segregation. Defect and Diffusion Forum, 2001, 188-190, 143-152.	0.4	0

#	Article	IF	Citations
55	Helix transition in di-block polyampholyte. Journal of Physics Condensed Matter, 2001, 13, 10279-10291.	0.7	18
56	A molecular dynamics study of the diffusion processes in liquid Na-K alloys. Journal of Physics Condensed Matter, 1999, 11, 1397-1408.	0.7	8
57	Theoretical and computer simulation study of density fluctuations in liquid binary alloys. European Physical Journal B, 1999, 7, 129-136.	0.6	7
58	Correction for finite-size effects in molecular dynamics simulation of liquid alloys. Journal of Non-Crystalline Solids, 1999, 250-252, 354-359.	1.5	5
59	Dynamical Properties of Liquid Binary Alloys: A Memory Function Study. Physics and Chemistry of Liquids, 1996, 32, 87-102.	0.4	27
60	On the Mechanism of Alkylammonium Ligands Binding to the Surface of CsPbBr3 Nanocrystals. , 0, , .		0