Pradipta Bandyopadhyay

List of Publications by Year
in descending order

41 papers	1,145 citations	623734 14 h-index	377865 34 g-index
41 all docs	41 docs citations	41 times ranked	1350 citing authors

#	Article	IF	Citations
1	Calcium Ion Binding to the Mutants of Calmodulin: A Structure-Based Computational Predictive Model of Binding Affinity Using a Charge Scaling Approach in Molecular Dynamics Simulation. Journal of Chemical Information and Modeling, 2022, 62, 2821-2834.	5.4	7
2	Calcium ion binding to calmodulin: binding free energy calculation using the molecular mechanics Poisson-Boltzmann surface area (MM-PBSA) method by incorporating implicit polarization. Journal of Biomolecular Structure and Dynamics, 2021, 39, 7213-7222.	3.5	18
3	Calculation of salt-dependent free energy of binding of Î²-lactoglobulin homodimer formation and mechanism of dimer formation using molecular dynamics simulation and three-dimensional reference interaction site model (3D-RISM): diffuse salt ions and non-polar interactions between the monomers favor the dimer formation. Physical Chemistry Chemical Physics, 2020, 22, 2142-2156.	2.8	6
4	A look inside the black box: Using graph-theoretical descriptors to interpret a Continuous-Filter Convolutional Neural Network (CF-CNN) trained on the global and local minimum energy structures of neutral water clusters. Journal of Chemical Physics, 2020, 153, 024302.	3.0	14
5	A comparative evaluation of pair correlation functions for a highly asymmetric electrolyte with mono and divalent counterions from integral equation theory in hypernetted chain (HNC) approximation and Monte Carlo simulation. Chemical Physics Letters, 2019, 732, 136664.	2.6	7
6	Atlas of putative minima and low-lying energy networks of water clusters n = 3â€“25. Journal of Chemical Physics, 2019, 151, 214307.	3.0	41
7	Comparison of molecular mechanics-Poisson-Boltzmann surface area (MM-PBSA) and molecular mechanics-three-dimensional reference interaction site model (MM-3D-RISM) method to calculate the binding free energy of protein-ligand complexes: Effect of metal ion and advance statistical test. Chemical Physics Letters, 2018, 695, 69-78.	2.6	17
8	Microscopic picture of water-ethylene glycol interaction near a model DNA by computer simulation: Concentration dependence, structure, and localized thermodynamics. PLoS ONE, 2018, 13, e0206359.	2.5	9
9	A memory-based random walk model to understand diffusion in crowded heterogeneous environment. International Journal of Modern Physics B, 2018, 32, 1850193.	2.0	1
10	Understanding the structure and hydrogen bonding network of (H₂O)₃₂ and (H₂O)₃₃: an improved Monte Carlo temperature basin paving (MCTBP) method and quantum theory of atoms in molecules (QTAIM) analysis. RSC Advances, 2017, 7, 18401-18417.	3.6	16
11	How Mg²⁺ ion and water network affect the stability and structure of non-Watsonâ€“Crick base pairs in E. coli loop E of 5S rRNA: a molecular dynamics and reference interaction site model (RISM) study. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2103-2122.	3.5	5
12	A combination of Monte Carlo Temperature Basin Paving and Graph theory: Water cluster low energy structures and completeness of search. Journal of Chemical Sciences, 2016, 128, 1507-1516.	1.5	1
13	Free Energy Contribution Analysis Using Response Kernel Approximation: Insights into the Acylation Reaction of a Beta-Lactamase. Journal of Physical Chemistry B, 2016, 120, 9338-9346.	2.6	6
14	Foldingâ€“unfolding transition in the mini-protein villin headpiece (HP35): An equilibrium study using the Wangâ€“Landau algorithm. Chemical Physics, 2016, 468, 1-8.	1.9	3
15	An analytical correlated random walk model and its application to understand subdiffusion in crowded environment. Journal of Chemical Physics, 2015, 143, 114104.	3.0	8
16	Low energy isomers of (H2O)25 from a hierarchical method based on Monte Carlo temperature basin paving and molecular tailoring approaches benchmarked by MP2 calculations. Journal of Chemical Physics, 2014, 141, 164304.	3.0	23
17	Interchain hydrophobic clustering promotes rigidity in HIV-1 protease flap dynamics: new insights from Molecular Dynamics. Journal of Biomolecular Structure and Dynamics, 2014, 32, 899-915.	3.5	3
18	Wang-Landau density of states based study of the folding-unfolding transition in the mini-protein Trp-cage (TC5b). Journal of Chemical Physics, 2014, 141, 015103.	3.0	3

#	Article	IF	Citations
19	A comparative Brownian dynamics investigation between small linear and circular DNA: Scaling of diffusion coefficient with size and topology of DNA. Chemical Physics Letters, 2014, 591, 253-258.	2.6	4
20	A New Coarse-Grained Model for E. coli Cytoplasm: Accurate Calculation of the Diffusion Coefficient of Proteins and Observation of Anomalous Diffusion. PLoS ONE, 2014, 9, e106466.	2.5	34
21	Finding low energy minima of (H2O)25 and (H2O)30 with temperature basin paving Monte Carlo method with effective fragment potential: New â€˜global minimumâ€™ and graph theoretical characterization of low energy structures. Computational and Theoretical Chemistry, 2013, 1021, 206-214.	2.5	14
22	Cooperative Roles of Charge Transfer and Dispersion Terms in Hydrogen-Bonded Networks of (H₂O)_n, n = 6, 11, and 16. Journal of Physical Chemistry A, 2013, 117, 6641-6651.	2.5	24
23	Increasing the efficiency of Monte Carlo simulation with sampling from an approximate potential. Chemical Physics Letters, 2013, 556, 341-345.	2.6	10
24	Accurate Calculation of the Density of States near the Ground-State Energy of the Peptides Met-Enkephalin and (Alanine)₅ with the Wang-Landau Method: Lessons Learned. Journal of Atomic, Molecular, and Optical Physics, 2012, 2012, 1-6.	0.5	2
25	Facilitating Minima Search for Large Water Clusters at the MP2 Level via Molecular Tailoring. Journal of Physical Chemistry Letters, 2012, 3, 2253-2258.	4.6	69
26	Determination of low-energy structures of a small RNA hairpin using Monte Carloâ€“based techniques. Journal of Biosciences, 2012, 37, 533-538.	1.1	2
27	Investigation of the acylation mechanism of class C beta-lactamase: pKa calculation, molecular dynamics simulation and quantum mechanical calculation. Journal of Molecular Modeling, 2012, 18, 481-492.	1.8	9
28	Monte Carlo Temperature Basin Paving with Effective Fragment Potential: An Efficient and Fast Method for Finding Low-Energy Structures of Water Clusters (H₂O)₂₀ and (H₂O)₂₅. Journal of Physical Chemistry A, 2011, 115, 11866-11875.	2.5	39
29	Understanding the applicability and limitations of Wangâ€“Landau method for biomolecules: Met-enkephalin and Trp-cage. Chemical Physics Letters, 2011, 514, 357-361.	2.6	8
30	Monte Carlo Energy Landscape Paving and Basin Paving simulation of RNA T-loop hairpin. Chemical Physics Letters, 2011, 502, 130-135.	2.6	4
31	Efficient conformational sampling by Monte Carlo Basin Paving method: Distribution of minima on the energy surface of (H2O)20 and (H2O)50. Chemical Physics Letters, 2010, 487, 133-138.	2.6	6
32	Riboswitch Detection Using Profile Hidden Markov Models. BMC Bioinformatics, 2009, 10, 325.	2.6	34
33	Computational investigation of kinetics of crossâ€linking reactions in proteins: Importance in structure prediction. Biopolymers, 2009, 91, 68-77.	2.4	1
34	Molecular dynamics simulation of HIV-protease with polarizable and non-polarizable force fields. Indian Journal of Physics, 2009, 83, 81-90.	1.8	7
35	Assessment of Two Surface Monte Carlo (TSMC) method to find stationary points of (H2O)15 and (H2O)20 clusters. Theoretical Chemistry Accounts, 2008, 120, 307-312.	1.4	15
36	Partial Acetylation of Lysine Residues Improves Intraprotein Cross-Linking. Analytical Chemistry, 2008, 80, 951-960.	6.5	34

#	Article	IF	Citations
37	Two-surface Monte Carlo with basin hopping: Quantum mechanical trajectory and multiple stationary points of water cluster. Journal of Chemical Physics, 2008, 128, 134103.	3.0	10
38	Drug Resistance of HIV-1 Protease Against JE-2147: I47V Mutation Investigated by Molecular Dynamics Simulation. Chemical Biology and Drug Design, 2006, 67, 155-161.	3.2	16
39	Accelerating quantum mechanical/molecular mechanical sampling using pure molecular mechanical potential as an importance function: The case of effective fragment potential. Journal of Chemical Physics, 2005, 122, 091102.	3.0	33
40	The Effective Fragment Potential Method:Â A QM-Based MM Approach to Modeling Environmental Effects in Chemistry. Journal of Physical Chemistry A, 2001, 105, 293-307.	2.5	570
41	Ab initioMonte Carlo simulation using multicanonical algorithm: temperature dependence of the average structure of water dimer. Molecular Physics, 1999, 96, 349-358.	1.7	12