# Jaydeep P Bardhan

List of Publications by Year
in descending order



| 35 | 624 | 706676 14 | 651938 25 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 35 | 35 | 35 | 544 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Guest Editor's Introduction: DOE Computational Science Graduate Fellowship Research Showcase. Computing in Science and Engineering, 2021, 23, 5-8. | 1.2 | 1 |
| 2 | Highâ€performance transformation of protein structure representation from internal to Cartesian coordinates. Journal of Computational Chemistry, 2020, 41, 2104-2114. | 1.5 | 3 |
| 3 | Solvation thermodynamics of neutral and charged solutes using the solvationâ€layer interface condition continuum dielectric model. International Journal of Quantum Chemistry, 2019, 119, e25771. | 1.0 | 5 |
| 4 | Predicting solvation free energies and thermodynamics in polar solvents and mixtures using a solvation-layer interface condition. Journal of Chemical Physics, 2017, 146, . | 1.2 | 14 |
| 5 | Extending the Solvation-Layer Interface Condition Continuum Electrostatic Model to a Linearized Poissonâ€“Boltzmann Solvent. Journal of Chemical Theory and Computation, 2017, 13, 2897-2914. | 2.3 | 7 |
| 6 | Effects of Catalytic Action and Ligand Binding on Conformational Ensembles of Adenylate Kinase. Biochemistry, 2017, 56, 4559-4567. | 1.2 | 13 |
| 7 | Theory of wavelet-based coarse-graining hierarchies for molecular dynamics. Physical Review E, 2017, 96, 013301. | 0.8 | 1 |
| 8 | Comparative Assessment of Nonlocal Continuum Solvent Models Exhibiting Overscreening. Computational and Mathematical Biophysics, 2017, 5, 40-57. | 0.6 | 2 |
| 9 | A framework to optimize protein structure from solution scattering using ADMM and an elastic subdomain network. , 2016, , . | | 1 |
| 10 | Generalising the mean spherical approximation as a multiscale, nonlinear boundary condition at the soluteâ€“solvent interface. Molecular Physics, 2016, 114, 2558-2567. | 0.8 | 6 |
| 11 | Nonlocal Electrostatics in Spherical Geometries Using Eigenfunction Expansions of Boundary-Integral Operators. Computational and Mathematical Biophysics, 2015, 3, 1-22. | 0.6 | 2 |
| 12 | Constrained Maximum Likelihood Estimation of Relative Abundances of Protein Conformation in a Heterogeneous Mixture From Small Angle X-Ray Scattering Intensity Measurements. IEEE Transactions on Signal Processing, 2015, 63, 5383-5394. | 3.2 | 10 |
| 13 | Diffusion Wavelet Decomposition for Coarse-Graining of Polymer Chains. Materials Research Society Symposia Proceedings, 2015, 1753, 24. | 0.1 | 0 |
| 14 | Accelerating protein coordinate conversion using GPUs. , 2014, , . | | 1 |
| 15 | Communication: Modeling charge-sign asymmetric solvation free energies with nonlinear boundary conditions. Journal of Chemical Physics, 2014, 141, 131103. | 1.2 | 23 |
| 16 | A biomolecular electrostatics solver using Python, GPUs and boundary elements that can handle solvent-filled cavities and Stern layers. Computer Physics Communications, 2014, 185, 720-729. | 3.0 | 33 |
| 17 | Gradient models in molecular biophysics: progress, challenges, opportunities. Journal of the Mechanical Behavior of Materials, 2013, 22, 169-184. | 0.7 | 11 |
| 18 | Analysis of fast boundary-integral approximations for modeling electrostatic contributions of molecular binding. Computational and Mathematical Biophysics, 2013, 1, 124-150. | 0.6 | 2 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Computational science and re-discovery: open-source implementation of ellipsoidal harmonics for problems in potential theory. Computational Science & Discovery, 2012, 5, 014006. | 1.5 | 7 |
| 20 | Comparison of three-dimensional Poisson solution methods for particle-based simulation and inhomogeneous dielectrics. Physical Review E, 2012, 86, 011912. | 0.8 | 22 |
| 21 | Biomolecular electrostaticsâ€"I want your solvation (model). Computational Science & Discovery, 2012, 5, 013001. | 1.5 | 30 |
| 22 | Affine-response model of molecular solvation of ions: Accurate predictions of asymmetric charging free energies. Journal of Chemical Physics, 2012, 137, 124101. | 1.2 | 40 |
| 23 | </title> </titles> <publication_dates> <month>06</month> <year>2012</year> </publication_date> <pages> <first_page>C2</first_page> <last_page>C2</last_page> </pages> <publisher_item> <item_number item_number_type='arNumber'>6327712</item_number> </publisher_item> <doi_data> <doi>10.1109/MDT.2012.2213176</doi> <resource>http://ieeexplore.ieee.org/lpdocs/epic03/wrapper.htm?arnumbe IEEE Design and Test of | 1.4 | 0 |
| 24 | Biomolecular electrostatics using a fast multipole BEM on up to 512 gpus and a billion unknowns. Computer Physics Communications, 2011, 182, 1272-1283. | 3.0 | 73 |
| 25 | Efficiently accounting for ion correlations in electrokinetic nanofluidic devices using density functional theory. Journal of Colloid and Interface Science, 2011, 359, 520-529. | 5.0 | 45 |
| 26 | Nonlocal continuum electrostatic theory predicts surprisingly small energetic penalties for charge burial in proteins. Journal of Chemical Physics, 2011, 135, 104113. | 1.2 | 23 |
| 27 | Mathematical analysis of the boundary-integral based electrostatics estimation approximation for molecular solvation: Exact results for spherical inclusions. Journal of Chemical Physics, 2011, 135, 124107. | 1.2 | 10 |
| 28 | Discretization of the induced-charge boundary integral equation. Physical Review E, 2009, 80, 011906. | 0.8 | 24 |
| 29 | Bounding the electrostatic free energies associated with linear continuum models of molecular solvation. Journal of Chemical Physics, 2009, 130, 104108. | 1.2 | 14 |
| 30 | Accurate solution of multiâ€•region continuum biomolecule electrostatic problems using the linearized Poissonâ€“Boltzmann equation with curved boundary elements. Journal of Computational Chemistry, 2009, 30, 132-153. | 1.5 | 80 |
| 31 | â€œReverse-Schurâ€•Approach to Optimization with Linear PDE Constraints: Application to Biomolecule Analysis and Design. Journal of Chemical Theory and Computation, 2009, 5, 3260-3278. | 2.3 | 8 |
| 32 | Numerical solution of boundary-integral equations for molecular electrostatics. Journal of Chemical Physics, 2009, 130, 094102. | 1.2 | 41 |
| 33 | Interpreting the Coulomb-field approximation for generalized-Born electrostatics using boundary-integral equation theory. Journal of Chemical Physics, 2008, 129, 144105. | 1.2 | 27 |
| 34 | Numerical integration techniques for curved-element discretizations of molecule-solvent interfaces. Journal of Chemical Physics, 2007, 127, 014701. | 1.2 | 33 |
| 35 | An Accurate Surface Formulation for Biomolecule Electrostatics in Non-Ionic Solutions. , 2005, 2005, 7591-5. | | 12 |