Qin Cai

List of Publications by Year
in descending order

18	712	567281 15	839539 18
papers	citations	h-index	g-index

18	18	18	522
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A semi-implicit augmented IIM for Navierâ€“Stokes equations with open, traction, or free boundary conditions. Journal of Computational Physics, 2015, 297, 182-193.	3.8	10
2	Biological applications of classical electrostatics methods. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440008.	1.8	16
3	A multi-scale method for dynamics simulation in continuum solvent models. I: Finite-difference algorithm for Navierâ€“Stokes equation. Chemical Physics Letters, 2014, 616-617, 67-74.	2.6	11
4	Numerical Poissonâ€“Boltzmann model for continuum membrane systems. Chemical Physics Letters, 2013, 555, 274-281.	2.6	26
5	Electrostatic forces in the Poisson-Boltzmann systems. Journal of Chemical Physics, 2013, 139, 094106.	3.0	27
6	Exploring accurate Poissonâ€“Boltzmann methods for biomolecular simulations. Computational and Theoretical Chemistry, 2013, 1024, 34-44.	2.5	35
7	Poissonâ€“Boltzmann Implicit Solvation Models. Annual Reports in Computational Chemistry, 2012, , 149-162.	1.7	12
8	Dielectric pressure in continuum electrostatic solvation of biomolecules. Physical Chemistry Chemical Physics, 2012, 14, 15917.	2.8	26
9	Reducing Grid Dependence in Finite-Difference Poissonâ€“Boltzmann Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2741-2751.	5.3	58
10	Development of Polarizable Models for Molecular Mechanical Calculations. 3. Polarizable Water Models Conforming to Thole Polarization Screening Schemes. Journal of Physical Chemistry B, 2012, 116, 7999-8008.	2.6	49
11	Development of Polarizable Models for Molecular Mechanical Calculations. 4. van der Waals Parametrization. Journal of Physical Chemistry B, 2012, 116, 7088-7101.	2.6	60
12	Development of Polarizable Models for Molecular Mechanical Calculations II: Induced Dipole Models Significantly Improve Accuracy of Intermolecular Interaction Energies. Journal of Physical Chemistry B, 2011, 115, 3100-3111.	2.6	116
13	On-the-Fly Numerical Surface Integration for Finite-Difference Poissonâ€“Boltzmann Methods. Journal of Chemical Theory and Computation, 2011, 7, 3608-3619.	5.3	24
14	Dielectric boundary force in numerical Poissonâ€“Boltzmann methods: Theory and numerical strategies. Chemical Physics Letters, 2011, 514, 368-373.	2.6	30
15	Performance of Nonlinear Finite-Difference Poissonâ^'Boltzmann Solvers. Journal of Chemical Theory and Computation, 2010, 6, 203-211.	5.3	89
16	On removal of charge singularity in Poissonâ€“Boltzmann equation. Journal of Chemical Physics, 2009, 130, 145101.	3.0	47
17	Achieving energy conservation in Poissonâ€“Boltzmann molecular dynamics: Accuracy and precision with finite-difference algorithms. Chemical Physics Letters, 2009, 468, 112-118.	2.6	50
18	Roles of Boundary Conditions in DNA Simulations: Analysis of Ion Distributions with the Finite-Difference Poisson-Boltzmann Method. Biophysical Journal, 2009, 97, 554-562.	0.5	26