Jay W Ponder

List of Publications by Year
in descending order

62 papers	12,246 citations	87886 38 h-index	123420 61 g-index
64 all docs	64 docs citations	64 times ranked	8782 citing authors

#	Article	IF	Citations
1	Force Fields for Protein Simulations. Advances in Protein Chemistry, 2003, 66, 27-85.	4.4	1,560
2	Tertiary templates for proteins. Journal of Molecular Biology, 1987, 193, 775-791.	4.2	1,496
3	Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation. Journal of Physical Chemistry B, 2003, 107, 5933-5947.	2.6	1,270
4	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	2.6	1,093
5	An efficient newton-like method for molecular mechanics energy minimization of large molecules. Journal of Computational Chemistry, 1987, 8, 1016-1024.	3.3	854
6	Consistent treatment of inter- and intramolecular polarization in molecular mechanics calculations. Journal of Computational Chemistry, 2002, 23, 1497-1506.	3.3	545
7	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4046-4063.	5.3	524
8	Ion Solvation Thermodynamics from Simulation with a Polarizable Force Field. Journal of the American Chemical Society, 2003, 125, 15671-15682.	13.7	474
9	Tinker 8: Software Tools for Molecular Design. Journal of Chemical Theory and Computation, 2018, 14, 5273-5289.	5.3	403
10	Polarizable Atomic Multipole-Based Molecular Mechanics for Organic Molecules. Journal of Chemical Theory and Computation, 2011, 7, 3143-3161.	5.3	385
11	Systematic Improvement of a Classical Molecular Model of Water. Journal of Physical Chemistry B, 2013, 117, 9956-9972.	2.6	279
12	Analysis and Application of Potential Energy Smoothing and Search Methods for Global Optimization. Journal of Physical Chemistry B, 1998, 102, 9725-9742.	2.6	239
13	Accurate modeling of the intramolecular electrostatic energy of proteins. Journal of Computational Chemistry, 1995, 16, 791-816.	3.3	228
14	Temperature and Pressure Dependence of the AMOEBA Water Model. Journal of Physical Chemistry B, 2004, 108, 13427-13437.	2.6	191
15	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. Chemical Science, 2018, 9, 956-972.	7.4	190
16	Algorithms for calculating excluded volume and its derivatives as a function of molecular conformation and their use in energy minimization. Journal of Computational Chemistry, 1991, 12, 402-409.	3.3	183
17	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. Journal of Physical Chemistry B, 2015, 119, 9423-9437.	2.6	183
18	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. Journal of Chemical Theory and Computation, 2018, 14, 2084-2108.	5.3	178

#	Article	IF	Citations
19	The NMR Solution Structure of Intestinal Fatty Acid-binding Protein Complexed with Palmitate: Application of a Novel Distance Geometry Algorithm. Journal of Molecular Biology, 1996, 264, 585-602.	4.2	159
20	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. Journal of Chemical Theory and Computation, 2015, 11, 2609-2618.	5.3	93
21	Ab Initio fold prediction of small helical proteins using distance geometry and knowledge-based scoring functions 1 1Edited by F. Cohen. Journal of Molecular Biology, 1999, 290, 267-281.	4.2	89
22	Tinker–OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. Journal of Computational Chemistry, 2017, 38, 2047-2055.	3.3	89
23	Protein structure prediction using a combination of sequence homology and global energy minimization: II. Energy functions. Journal of Computational Chemistry, 1998, 19, 548-573.	3.3	83
24	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. International Journal of Quantum Chemistry, 2007, 107, 1390-1395.	2.0	81
25	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. Journal of Chemical Physics, 2007, 126, 124114.	3.0	79
26	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	2.6	77
27	Multipole electrostatics in hydration free energy calculations. Journal of Computational Chemistry, 2011, 32, 967-977.	3.3	69
28	Polarizable Atomic Multipole Solutes in a Generalized Kirkwood Continuum. Journal of Chemical Theory and Computation, 2007, 3, 2083-2097.	5.3	66
29	An optimized charge penetration model for use with the AMOEBA force field. Physical Chemistry Chemical Physics, 2017, 19, 276-291.	2.8	65
30	Stereochemistry of the hygrolidins. Tetrahedron Letters, 1984, 25, 4325-4328.	1.4	59
31	A potential smoothing algorithm accurately predicts transmembrane helix packing. Nature Structural Biology, 1999, 6, 50-55.	9.7	57
32	Calculation of the reaction field due to off-center point multipoles. Journal of Chemical Physics, 1997, 107, 481-492.	3.0	55
33	Classical Pauli repulsion: An anisotropic, atomic multipole model. Journal of Chemical Physics, 2019, 150, 084104.	3.0	51
34	The structure and dynamics of rat apo-cellular retinol-binding protein II in solution: comparison with the X-ray structure 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1999, 286, 1179-1195.	4.2	46
35	TINKTEP: A fully self-consistent, mutually polarizable QM/MM approach based on the AMOEBA force field. Journal of Chemical Physics, 2016, 145, 124106.	3.0	46
36	Binding of retinol induces changes in rat cellular retinol-binding protein II conformation and backbone dynamics. Journal of Molecular Biology, 2000, 300, 619-632.	4.2	44

#	Article	IF	Citations
37	Calculating binding free energies of host–guest systems using the AMOEBA polarizable force field. Physical Chemistry Chemical Physics, 2016, 18, 30261-30269.	2.8	44
38	Accuracy of side-chain prediction upon near-native protein backbones generated by ab initio folding methods. , 1998, 33, 204-217.		42
39	MSCALE: A General Utility for Multiscale Modeling. Journal of Chemical Theory and Computation, 2011, 7, 1208-1219.	5.3	41
40	Tinker-HP: Accelerating Molecular Dynamics Simulations of Large Complex Systems with Advanced Point Dipole Polarizable Force Fields Using GPUs and Multi-GPU Systems. Journal of Chemical Theory and Computation, 2021, 17, 2034-2053.	5.3	40
41	The stereochemistry and biosynthesis of hybridalactone, an eicosanoid from. Tetrahedron Letters, 1984, 25, 1015-1018.	1.4	36
42	A valence bond model for aqueous Cu(II) and Zn(II) ions in the AMOEBA polarizable force field. Journal of Computational Chemistry, 2013, 34, 739-749.	3.3	34
43	Truncated Conjugate Gradient: An Optimal Strategy for the Analytical Evaluation of the Many-Body Polarization Energy and Forces in Molecular Simulations. Journal of Chemical Theory and Computation, 2017, 13, 180-190.	5.3	34
44	Exploring the similarities between potential smoothing and simulated annealing. Journal of Computational Chemistry, 2000, 21, 531-552.	3.3	30
45	Molecular Dynamics of β-Hairpin Models of Epigenetic Recognition Motifs. Journal of the American Chemical Society, 2012, 134, 15970-15978.	13.7	29
46	An Angular Overlap Model for Cu(II) Ion in the AMOEBA Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 298-311.	5.3	28
47	An empirical extrapolation scheme for efficient treatment of induced dipoles. Journal of Chemical Physics, 2016, 145, 164101.	3.0	27
48	Distance geometry generates native–like folds for small helical proteins using the consensus distances of predicted protein structures. Protein Science, 1998, 7, 1998-2003.	7.6	26
49	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. Journal of Chemical Theory and Computation, 2015, 11, 5326-5339.	5.3	26
50	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short–range penetration correction up to quadrupoles. Journal of Computational Chemistry, 2016, 37, 494-506.	3.3	26
51	Absolute binding free energies for the SAMPL6 cucurbit[8]uril host–guest challenge via the AMOEBA polarizable force field. Journal of Computer-Aided Molecular Design, 2018, 32, 1087-1095.	2.9	26
52	Polarizable Water Potential Derived from a Model Electron Density. Journal of Chemical Theory and Computation, 2021, 17, 7056-7084.	5.3	26
53	High-Resolution Crystal Structures of Protein Helices Reconciled with Three-Centered Hydrogen Bonds and Multipole Electrostatics. PLoS ONE, 2015, 10, e0123146.	2.5	25
54	AMOEBA binding free energies for the SAMPL7 TrimerTrip host–guest challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 79-93.	2.9	21

#	Article	IF	Citations
55	Computationally driven discovery of SARS-CoV-2 M^{pro}inhibitors: from design to experimental validation. Chemical Science, 2022, 13, 3674-3687.	7.4	21
56	A physically grounded damped dispersion model with particle mesh Ewald summation. Journal of Chemical Physics, 2018, 149, 084115.	3.0	18
57	Crystallization and Initial X-ray Crystallographic Characterization of Recombinant Bovine Inositol Polyphosphate 1-Phosphatase Produced in Spodoptera frugiperda Cells. Journal of Molecular Biology, 1994, 236, 584-589.	4.2	16
58	Helix stability of oligoglycine, oligoalanine, and oligo-Î²-alanine dodecamers reflected by hydrogen-bond persistence. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3043-3061.	2.6	15
59	Metal-ammonia reduction of triptycene and related benzobarrelene derivatives. Journal of Organic Chemistry, 1979, 44, 4594-4597.	3.2	10
60	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. Journal of Chemical Theory and Computation, 2021, 17, 2323-2341.	5.3	10
61	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	8
62	Protein structure prediction using a combination of sequence homology and global energy minimization: II. Energy functions. Journal of Computational Chemistry, 1998, 19, 548.	3.3	4