Jay W Ponder

List of Publications by Year in Descending Order

62 papers	10,407 citations	37 h-index	64 g-index
64 ext. papers	11,272 ext. citations	5.1 avg, IF	6.32 L-index

#	Paper	IF	Citations
62	Computationally driven discovery of SARS-CoV-2 M inhibitors: from design to experimental validation.. *Chemical Science*, **2022**, 13, 3674-3687	9.4	2
61	Polarizable Water Potential Derived from a Model Electron Density. *Journal of Chemical Theory and Computation*, **2021**, 17, 7056-7084	6.4	5
60	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	6.4	11
59	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. *Journal of Chemical Theory and Computation*, **2021**, 17, 2323-2341	6.4	5
58	AMOEBA binding free energies for the SAMPL7 TrimerTrip host-guest challenge. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 79-93	4.2	8
57	Classical Pauli repulsion: An anisotropic, atomic multipole model. *Journal of Chemical Physics*, **2019**, 150, 084104	3.9	30
56	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	7
55	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. *Journal of Chemical Theory and Computation*, **2018**, 14, 2084-2108	6.4	122
54	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	9.4	122
53	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	4.2	18
52	Tinker 8: Software Tools for Molecular Design. *Journal of Chemical Theory and Computation*, **2018**, 14, 5273-5289	6.4	188
51	A physically grounded damped dispersion model with particle mesh Ewald summation. *Journal of Chemical Physics*, **2018**, 149, 084115	3.9	13
50	Tinker-OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. *Journal of Computational Chemistry*, **2017**, 38, 2047-2055	3.5	70
49	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	6.4	28
48	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	3.5	26
47	An optimized charge penetration model for use with the AMOEBA force field. *Physical Chemistry Chemical Physics*, **2016**, 19, 276-291	3.6	43
46	An empirical extrapolation scheme for efficient treatment of induced dipoles. *Journal of Chemical Physics*, **2016**, 145, 164101	3.9	24

45	TINKTEP: A fully self-consistent, mutually polarizable QM/MM approach based on the AMOEBA force field. *Journal of Chemical Physics*, **2016**, 145, 124106	3.9	38
44	Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field. *Physical Chemistry Chemical Physics*, **2016**, 18, 30261-30269	3.6	36
43	Advanced Potential Energy Surfaces for Molecular Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 9811-32	3.4	66
42	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. *Journal of Chemical Theory and Computation*, **2015**, 11, 5326-39	6.4	17
41	High-resolution crystal structures of protein helices reconciled with three-centered hydrogen bonds and multipole electrostatics. *PLoS ONE*, **2015**, 10, e0123146	3.7	20
40	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. *Journal of Chemical Theory and Computation*, **2015**, 11, 2609-2618	6.4	79
39	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. *Journal of Physical Chemistry B*, **2015**, 119, 9423-9437	3.4	149
38	An Angular Overlap Model for Cu(II) Ion in the AMOEBA Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 298-311	6.4	25
37	Helix stability of oligoglycine, oligoalanine, and oligo-β-alanine dodecamers reflected by hydrogen-bond persistence. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 3043-61	4.2	12
36	The Polarizable Atomic Multipole-based AMOEBA Force Field for Proteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 4046-4063	6.4	409
35	Systematic improvement of a classical molecular model of water. *Journal of Physical Chemistry B*, **2013**, 117, 9956-72	3.4	235
34	A valence bond model for aqueous Cu(II) and Zn(II) ions in the AMOEBA polarizable force field. *Journal of Computational Chemistry*, **2013**, 34, 739-49	3.5	29
33	Molecular dynamics of β-hairpin models of epigenetic recognition motifs. *Journal of the American Chemical Society*, **2012**, 134, 15970-8	16.4	27
32	MSCALE: A General Utility for Multiscale Modeling. *Journal of Chemical Theory and Computation*, **2011**, 7, 1208-1219	6.4	38
31	Multipole electrostatics in hydration free energy calculations. *Journal of Computational Chemistry*, **2011**, 32, 967-77	3.5	60
30	Polarizable Atomic Multipole-based Molecular Mechanics for Organic Molecules. *Journal of Chemical Theory and Computation*, **2011**, 7, 3143-3161	6.4	320
29	Current status of the AMOEBA polarizable force field. *Journal of Physical Chemistry B*, **2010**, 114, 2549-64	3.4	914
28	Polarizable Atomic Multipole Solutes in a Generalized Kirkwood Continuum. *Journal of Chemical Theory and Computation*, **2007**, 3, 2083-97	6.4	60

27	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. *International Journal of Quantum Chemistry*, **2007**, 107, 1390-1395	2.1	75
26	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. *Journal of Chemical Physics*, **2007**, 126, 124114	3.9	74
25	Temperature and Pressure Dependence of the AMOEBA Water Model. *Journal of Physical Chemistry B*, **2004**, 108, 13427-13437	3.4	175
24	Ion solvation thermodynamics from simulation with a polarizable force field. *Journal of the American Chemical Society*, **2003**, 125, 15671-82	16.4	430
23	Force fields for protein simulations. *Advances in Protein Chemistry*, **2003**, 66, 27-85		1303
22	Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation. *Journal of Physical Chemistry B*, **2003**, 107, 5933-5947	3.4	1148
21	Consistent treatment of inter- and intramolecular polarization in molecular mechanics calculations. *Journal of Computational Chemistry*, **2002**, 23, 1497-506	3.5	498
20	Exploring the similarities between potential smoothing and simulated annealing. *Journal of Computational Chemistry*, **2000**, 21, 531-552	3.5	28
19	Binding of retinol induces changes in rat cellular retinol-binding protein II conformation and backbone dynamics. *Journal of Molecular Biology*, **2000**, 300, 619-32	6.5	43
18	A potential smoothing algorithm accurately predicts transmembrane helix packing. *Nature Structural Biology*, **1999**, 6, 50-5		54
17	The structure and dynamics of rat apo-cellular retinol-binding protein II in solution: comparison with the X-ray structure. *Journal of Molecular Biology*, **1999**, 286, 1179-95	6.5	44
16	Ab initio fold prediction of small helical proteins using distance geometry and knowledge-based scoring functions. *Journal of Molecular Biology*, **1999**, 290, 267-81	6.5	76
15	Protein structure prediction using a combination of sequence homology and global energy minimization: II. Energy functions. *Journal of Computational Chemistry*, **1998**, 19, 548-573	3.5	80
14	Accuracy of side-chain prediction upon near-native protein backbones generated by Ab initio folding methods. *Proteins: Structure, Function and Bioinformatics*, **1998**, 33, 204-17	4.2	39
13	Distance geometry generates native-like folds for small helical proteins using the consensus distances of predicted protein structures. *Protein Science*, **1998**, 7, 1998-2003	6.3	22
12	Analysis and Application of Potential Energy Smoothing and Search Methods for Global Optimization. *Journal of Physical Chemistry B*, **1998**, 102, 9725-9742	3.4	229
11	Protein structure prediction using a combination of sequence homology and global energy minimization: II. Energy functions **1998**, 19, 548		4
10	Calculation of the reaction field due to off-center point multipoles. *Journal of Chemical Physics*, **1997**, 107, 481-492	3.9	53

9	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	6.5	143
8	Accurate modeling of the intramolecular electrostatic energy of proteins. *Journal of Computational Chemistry*, **1995**, 16, 791-816	3.5	207
7	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, 584-9	6.5	14
6	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	3.5	169
5	Tertiary templates for proteins. Use of packing criteria in the enumeration of allowed sequences for different structural classes. *Journal of Molecular Biology*, **1987**, 193, 775-91	6.5	1366
4	An efficient newton-like method for molecular mechanics energy minimization of large molecules. *Journal of Computational Chemistry*, **1987**, 8, 1016-1024	3.5	785
3	The stereochemistry and biosynthesis of hybridalactone, an eicosanoid from. *Tetrahedron Letters*, **1984**, 25, 1015-1018	2	35
2	Stereochemistry of the hygrolidins. *Tetrahedron Letters*, **1984**, 25, 4325-4328	2	50
1	Metal-ammonia reduction of triptycene and related benzobarrelene derivatives. *Journal of Organic Chemistry*, **1979**, 44, 4594-4597	4.2	7