Jean-Philip Piquemal

List of Publications by Year
in descending order

160 papers	10,916 citations	41323 49 h-index	33869 99 g-index
190 all docs	190 docs citations	190 times ranked	8684 citing authors

#	Article	IF	Citations
1	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	2.3	2,897
2	Are Bond Critical Points Really Critical for Hydrogen Bonding?. Journal of Chemical Theory and Computation, 2013, 9, 3263-3266.	2.3	414
3	Tinker 8: Software Tools for Molecular Design. Journal of Chemical Theory and Computation, 2018, 14, 5273-5289.	2.3	403
4	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	23.0	386
5	Anisotropic, Polarizable Molecular Mechanics Studies of Inter- and Intramolecular Interactions and Ligandâ^'Macromolecule Complexes. A Bottom-Up Strategy. Journal of Chemical Theory and Computation, 2007, 3, 1960-1986.	2.3	312
6	The Independent Gradient Model: A New Approach for Probing Strong and Weak Interactions in Molecules from Wave Function Calculations. ChemPhysChem, 2018, 19, 724-735.	1.0	263
7	Polarizable Force Fields for Biomolecular Simulations: Recent Advances and Applications. Annual Review of Biophysics, 2019, 48, 371-394.	4.5	253
8	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.	3.7	190
9	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. Journal of Chemical Theory and Computation, 2018, 14, 2084-2108.	2.3	178
10	Towards a force field based on density fitting. Journal of Chemical Physics, 2006, 124, 104101.	1.2	175
11	Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. Journal of Chemical Physics, 2006, 125, 054511.	1.2	169
12	Unraveling non-covalent interactions within flexible biomolecules: from electron density topology to gas phase spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 9876.	1.3	156
13	NCIPLOT4: Fast, Robust, and Quantitative Analysis of Noncovalent Interactions. Journal of Chemical Theory and Computation, 2020, 16, 4150-4158.	2.3	151
14	Polarizable Molecular Dynamics Simulation of Zn(II) in Water Using the AMOEBA Force Field. Journal of Chemical Theory and Computation, 2010, 6, 2059-2070.	2.3	137
15	A QM/MM Approach Using the AMOEBA Polarizable Embedding: From Ground State Energies to Electronic Excitations. Journal of Chemical Theory and Computation, 2016, 12, 3654-3661.	2.3	136
16	Improved Formulas for the Calculation of the Electrostatic Contribution to the Intermolecular Interaction Energy from Multipolar Expansion of the Electronic Distribution. Journal of Physical Chemistry A, 2003, 107, 10353-10359.	1.1	135
17	New Way for Probing Bond Strength. Journal of Physical Chemistry A, 2020, 124, 1850-1860.	1.1	121
18	Toward a Separate Reproduction of the Contributions to the Hartreeâ^'Fock and DFT Intermolecular Interaction Energies by Polarizable Molecular Mechanics with the SIBFA Potential. Journal of Chemical Theory and Computation, 2007, 3, 824-837.	2.3	104

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19	Coupling Quantum Interpretative Techniques: Another Look at Chemical Mechanisms in Organic Reactions. Journal of Chemical Theory and Computation, 2012, 8, 3993-3997.	2.3	104
20	Interpretation of the reduced density gradient. Molecular Physics, 2016, 114, 1406-1414.	0.8	103
21	Generalization of the Gaussian electrostatic model: Extension to arbitrary angular momentum, distributed multipoles, and speedup with reciprocal space methods. Journal of Chemical Physics, 2006, 125, 184101.	1.2	100
22	Modeling Structural Coordination and Ligand Binding in Zinc Proteins with a Polarizable Potential. Journal of Chemical Theory and Computation, 2012, 8, 1314-1324.	2.3	100
23	A CSOV study of the difference between HF and DFT intermolecular interaction energy values: The importance of the charge transfer contribution. Journal of Computational Chemistry, 2005, 26, 1052-1062.	1.5	99
24	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. Journal of Chemical Theory and Computation, 2015, 11, 2609-2618.	2.3	93
25	Tinkerâ€¢OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. Journal of Computational Chemistry, 2017, 38, 2047-2055.	1.5	89
26	AMOEBA+ Classical Potential for Modeling Molecular Interactions. Journal of Chemical Theory and Computation, 2019, 15, 4122-4139.	2.3	89
27	Gas-Phase Folding of a Two-Residue Model Peptide Chain: On the Importance of an Interplay between Experiment and Theory. Journal of the American Chemical Society, 2010, 132, 11860-11863.	6.6	83
28	Revealing strong interactions with the reduced density gradient: a benchmark for covalent, ionic and charge-shift bonds. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	82
29	Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. Journal of Chemical Theory and Computation, 2017, 13, 4025-4033.	2.3	81
30	Representation of Zn(II) complexes in polarizable molecular mechanics. Further refinements of the electrostatic and short-range contributions. Comparisons with parallelab initiocomputations. Journal of Computational Chemistry, 2005, 26, 1113-1130.	1.5	79
31	Gaussian Multipole Model (GMM). Journal of Chemical Theory and Computation, 2010, 6, 190-202.	2.3	79
32	Key Role of the Polarization Anisotropy of Water in Modeling Classical Polarizable Force Fields. Journal of Physical Chemistry A, 2007, 111, 8170-8176.	1.1	76
33	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: I. Toward Massively Parallel Direct Space Computations. Journal of Chemical Theory and Computation, 2014, 10, 1638-1651.	2.3	76
34	Modeling Organochlorine Compounds and the Ïƒ-Hole Effect Using a Polarizable Multipole Force Field. Journal of Physical Chemistry B, 2014, 118, 6456-6465.	1.2	69
35	<scp>LICHEM</scp>: A <scp>QM</scp>/<scp>MM</scp> program for simulations with multipolar and polarizable force fields. Journal of Computational Chemistry, 2016, 37, 1019-1029.	1.5	68
36	Inclusion of the ligand field contribution in a polarizable molecular mechanics: SIBFA-LF. Journal of Computational Chemistry, 2003, 24, 1963-1970.	1.5	65

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37	An optimized charge penetration model for use with the AMOEBA force field. Physical Chemistry Chemical Physics, 2017, 19, 276-291.	1.3	65
38	GEM*: A Molecular Electronic Density-Based Force Field for Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 1361-1365.	2.3	64
39	Characterizing Molecular Interactions in Chemical Systems. IEEE Transactions on Visualization and Computer Graphics, 2014, 20, 2476-2485.	2.9	63
40	Toward accurate solvation dynamics of lanthanides and actinides in water using polarizable force fields: from gas-phase energetics to hydration free energies. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	62
41	Advancing beyond charge analysis using the electronic localization function: Chemically intuitive distribution of electrostatic moments. Journal of Computational Chemistry, 2008, 29, 1440-1449.	1.5	60
42	Specificity of Acyl Transfer from 2-Mercaptobenzamide Thioesters to the HIV-1 Nucleocapsid Protein. Journal of the American Chemical Society, 2007, 129, 11067-11078.	6.6	56
43	Understanding Selectivity of Hard and Soft Metal Cations within Biological Systems Using the Subvalence Concept. 1. Application to Blood Coagulation: Direct Cationâ^'Protein Electronic Effects versus Indirect Interactions through Water Networks. Journal of Chemical Theory and Computation, 2010, 6, 1048-1063.	2.3	56
44	<scp>NCIPLOT</scp> and the analysis of noncovalent interactions using the reduced density gradient. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1497.	6.2	56
45	Intermolecular electrostatic energies using density fitting. Journal of Chemical Physics, 2005, 123, 044109.	1.2	55
46	Quantum Mechanics/Molecular Mechanics Electrostatic Embedding with Continuous and Discrete Functions. Journal of Physical Chemistry B, 2006, 110, 13682-13684.	1.2	53
47	Simple formulas for improved pointâ€charge electrostatics in classical force fields and hybrid quantum mechanical/molecular mechanical embedding. International Journal of Quantum Chemistry, 2008, 108, 1905-1912.	1.0	53
48	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II. Toward Massively Parallel Computations Using Smooth Particle Mesh Ewald. Journal of Chemical Theory and Computation, 2015, 11, 2589-2599.	2.3	53
49	Fragment-Localized Kohnâ^'Sham Orbitals via a Singles Configuration-Interaction Procedure and Application to Local Properties and Intermolecular Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2008, 4, 2020-2029.	2.3	51
50	Polarizable Water Molecules in Ligandâ^'Macromolecule Recognition. Impact on the Relative Affinities of Competing Pyrrolopyrimidine Inhibitors for FAK Kinase. Journal of the American Chemical Society, 2010, 132, 3312-3320.	6.6	51
51	Toward a Deeper Understanding of Enzyme Reactions Using the Coupled ELF/NCI Analysis: Application to DNA Repair Enzymes. Journal of Chemical Theory and Computation, 2013, 9, 2156-2160.	2.3	48
52	Complexes of thiomandelate and captopril mercaptocarboxylate inhibitors to metallo-Î²-lactamase by polarizable molecular mechanics. Validation on model binding sites by quantum chemistry. Journal of Computational Chemistry, 2005, 26, 1131-1147.	1.5	47
53	Quantum, classical, and hybrid QM/MM calculations in solution: General implementation of the ddCOSMO linear scaling strategy. Journal of Chemical Physics, 2014, 141, 184108.	1.2	47
54	Accurate Biomolecular Simulations Account for Electronic Polarization. Frontiers in Molecular Biosciences, 2019, 6, 143.	1.6	46

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55	Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. Journal of Chemical Theory and Computation, 2015, 11, 623-634.	2.3	45
56	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. Chemical Science, 2019, 10, 7200-7211.	3.7	45
57	Binding of 5-phospho-D-arabinonohydroxamate and 5-phospho-D-arabinonate inhibitors to zinc phosphomannose isomerase fromCandida albicans studied by polarizable molecular mechanics and quantum mechanics. Journal of Computational Chemistry, 2007, 28, 938-957.	1.5	44
58	DFT-steric-based energy decomposition analysis of intermolecular interactions. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	43
59	Implementation of Geometry-Dependent Charge Flux into the Polarizable AMOEBA+ Potential. Journal of Physical Chemistry Letters, 2020, 11, 419-426.	2.1	43
60	Revisiting the geometry of nd10 (n+1)s0 [M(H2O)]p+ complexes using four-component relativistic DFT calculations and scalar relativistic correlated CSOV energy decompositions (Mp+ = Cu+, Zn2+, Ag+,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.1	41
61	Ionic interactions: Comparative topological approach. Computational and Theoretical Chemistry, 2012, 998, 193-201.	1.1	41
62	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.	2.3	40
63	Understanding Lead Chemistry from Topological Insights: The Transition between Holoâ€•and Hemidirected Structures within the [Pb(CO)_n]²⁺ Model Series. Chemistry - A European Journal, 2008, 14, 2730-2743.	1.7	38
64	QM/MM Simulations with the Gaussian Electrostatic Model: A Density-based Polarizable Potential. Journal of Physical Chemistry Letters, 2018, 9, 3062-3067.	2.1	37
65	Numerical Fitting of Molecular Properties to Hermite Gaussians. Journal of Physical Chemistry A, 2007, 111, 12049-12056.	1.1	36
66	Hydration gibbs free energies of open and closed shell trivalent lanthanide and actinide cations from polarizable molecular dynamics. Journal of Molecular Modeling, 2014, 20, 2471.	0.8	35
67	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.	2.3	34
68	Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach. Journal of Physical Chemistry Letters, 2014, 5, 953-958.	2.1	32
69	Polarizable Water Networks in Ligandâ€“Metalloprotein Recognition. Impact on the Relative Complexation Energies of Zn-Dependent Phosphomannose Isomerase with <scp>d</scp>-Mannose 6-Phosphate Surrogates. Journal of Physical Chemistry B, 2011, 115, 8304-8316.	1.2	31
70	High-resolution mining of the SARS-CoV-2 main protease conformational space: supercomputer-driven unsupervised adaptive sampling. Chemical Science, 2021, 12, 4889-4907.	3.7	31
71	Manyâ€body exchangeâ€repulsion in polarizable molecular mechanics. I. orbitalâ€based approximations and applications to hydrated metal cation complexes. Journal of Computational Chemistry, 2011, 32, 2949-2957.	1.5	30
72	[Pb(H2O)]2+ and [Pb(OH)]+: Four-component density functional theory calculations, correlated scalar relativistic constrained-space orbital variation energy decompositions, and topological analysis. Journal of Chemical Physics, 2006, 124, 174311.	1.2	29

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73	Synthesis and structureâ€“activity relationship of non-peptidic antagonists of neuropilin-1 receptor. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4254-4259.	1.0	29
74	New intermolecular benchmark calculations on the water dimer: SAPT and supermolecular postâ€Hartreeâ€“Fock approaches. International Journal of Quantum Chemistry, 2009, 109, 3259-3267.	1.0	27
75	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general shortâ€range penetration correction up to quadrupoles. Journal of Computational Chemistry, 2016, 37, 494-506.	1.5	26
76	Capturing Many-Body Interactions with Classical Dipole Induction Models. Journal of Chemical Theory and Computation, 2017, 13, 2751-2761.	2.3	26
77	Pushing the Limits of Multiple-Time-Step Strategies for Polarizable Point Dipole Molecular Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 2593-2599.	2.1	25
78	The reaction mechanism of type I phosphomannose isomerases: New information from inhibition and polarizable molecular mechanics studies. Proteins: Structure, Function and Bioinformatics, 2011, 79, 203-220.	1.5	24
79	A Complete NCI Perspective: From New Bonds to Reactivity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 491-527.	0.6	24
80	Energy Analysis of Zn Polycoordination in a Metalloprotein Environment and of the Role of a Neighboring Aromatic Residue. What Is the Impact of Polarization?. Journal of Chemical Theory and Computation, 2008, 4, 1659-1668.	2.3	23
81	Synthesis and evaluation of non-hydrolyzable d-mannose 6-phosphate surrogates reveal 6-deoxy-6-dicarboxymethyl-d-mannose as a new strong inhibitor of phosphomannose isomerases. Bioorganic and Medicinal Chemistry, 2009, 17, 7100-7107.	1.4	23
82	Entasis through Hook-and-Loop Fastening in a Glycoligand with Cumulative Weak Forces Stabilizing Cu^I. Journal of the American Chemical Society, 2015, 137, 1141-1146.	6.6	23
83	S/G-1: An ab Initio Force-Field Blending Frozen Hermite Gaussian Densities and Distributed Multipoles. Proof of Concept and First Applications to Metal Cations. Journal of Physical Chemistry A, 2014, 118, 7598-7612.	1.1	22
84	Could an anisotropic molecular mechanics/dynamics potential account for sigma hole effects in the complexes of halogenated compounds?. Journal of Computational Chemistry, 2013, 34, 1125-1135.	1.5	21
85	A supervised fitting approach to force field parametrization with application to the SIBFA polarizable force field. Journal of Computational Chemistry, 2014, 35, 1577-1591.	1.5	21
86	Computationally driven discovery of SARS-CoV-2 M^{pro}inhibitors: from design to experimental validation. Chemical Science, 2022, 13, 3674-3687.	3.7	21
87	Channeling through Two Stacked Guanine Quartets of One and Two Alkali Cations in the Li⁺, Na⁺, K⁺, and Rb⁺ Series. Assessment of the Accuracy of the SIBFA Anisotropic Polarizable Molecular Mechanics Potential. Journal of Physical Chemistry B, 2017, 121, 3997-4014.	1.2	20
88	Elucidating the Phosphate Binding Mode of Phosphate-Binding Protein: The Critical Effect of Buffer Solution. Journal of Physical Chemistry B, 2018, 122, 6371-6376.	1.2	20
89	Massively Parallel Implementation of Steered Molecular Dynamics in Tinker-HP: Comparisons of Polarizable and Non-Polarizable Simulations of Realistic Systems. Journal of Chemical Theory and Computation, 2019, 15, 3694-3709.	2.3	20
90	Assessment of SAPT and Supermolecular EDA Approaches for the Development of Separable and Polarizable Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 2759-2774.	2.3	20

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91	Comments on the nature of the bonding in oxygenated dinuclear copper enzyme models. Computational and Theoretical Chemistry, 2006, 764, 77-86.	1.5	19
92	Role of Cation Polarization in holo- and hemi-Directed [Pb(H2O)n]2+ Complexes and Development of a Pb2+ Polarizable Force Field. Journal of Chemical Theory and Computation, 2011, 7, 138-147.	2.3	19
93	Stacked and H-Bonded Cytosine Dimers. Analysis of the Intermolecular Interaction Energies by Parallel Quantum Chemistry and Polarizable Molecular Mechanics.. Journal of Physical Chemistry B, 2015, 119, 9477-9495.	1.2	19
94	Analysis of the Interactions Taking Place in the Recognition Site of a Bimetallic Mg(II)â^'Zn(II) Enzyme, Isopentenyl Diphosphate Isomerase. A Parallel Quantum-Chemical and Polarizable Molecular Mechanics Study. Journal of Physical Chemistry B, 2010, 114, 4884-4895.	1.2	18
95	Correlation between electron localization and metal ion mutagenicity in DNA synthesis from QM/MM calculations. Physical Chemistry Chemical Physics, 2011, 13, 11239.	1.3	18
96	The truncated conjugate gradient (TCG), a non-iterative/fixed-cost strategy for computing polarization in molecular dynamics: Fast evaluation of analytical forces. Journal of Chemical Physics, 2017, 147, 161724.	1.2	18
97	Design Of Next Generation Force Fields From AB Initio Computations: Beyond Point Charges Electrostatics. Challenges and Advances in Computational Chemistry and Physics, 2009, , 137-172.	0.6	18
98	Electron Pair Localization Function (EPLF) for Density Functional Theory andab InitioWave Function-Based Methods: A New Tool for Chemical Interpretation. Journal of Chemical Theory and Computation, 2011, 7, 618-624.	2.3	17
99	How to make continuum solvation incredibly fast in a few simple steps: A practical guide to the domain decomposition paradigm for the conductorâ€like screening model. International Journal of Quantum Chemistry, 2019, 119, e25669.	1.0	17
100	Atomistic Polarizable Embeddings: Energy, Dynamics, Spectroscopy, and Reactivity. Accounts of Chemical Research, 2021, 54, 2812-2822.	7.6	17
101	Nuclear Quantum Effects in Liquid Water at Near Classical Computational Cost Using the Adaptive Quantum Thermal Bath. Journal of Physical Chemistry Letters, 2021, 12, 8285-8291.	2.1	17
102	Towards energy decomposition analysis for open and closed shell f-elements mono aqua complexes. Chemical Physics Letters, 2013, 563, 25-29.	1.2	16
103	Beyond holo/hemidirectionality in Pb(II) complexes: Can the valence lone pair be bisdirected?. Chemical Physics Letters, 2009, 478, 17-19.	1.2	14
104	Enforcing hemidirectionality in Pb(II) complexes: The importance of anionic ligands. Chemical Physics Letters, 2011, 510, 27-30.	1.2	14
105	Spinâ€driven activation of dioxygen in various metalloenzymes and their inspired models. Journal of Computational Chemistry, 2011, 32, 1178-1182.	1.5	14
106	Substituent-Modulated Affinities of Halobenzene Derivatives to the HIV-1 Integrase Recognition Site. Analyses of the Interaction Energies by Parallel Quantum Chemical and Polarizable Molecular Mechanics. Journal of Physical Chemistry A, 2014, 118, 9772-9782.	1.1	14
107	Could the â€œJanusâ€likeâ€•properties of the halobenzene CX bond (Xï£¾Cl, Br) be leveraged to enhance molecular recognition?. Journal of Computational Chemistry, 2015, 36, 210-221.	1.5	14
108	Theoretical study of phenol and 2-aminophenol docking at a model of the tyrosinase active site. New Journal of Chemistry, 2003, 27, 909.	1.4	13

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109	Importance of lone pair interactions/redistribution in hard and soft ligands within the active site of alcohol dehydrogenase Zn-metalloenzyme: Insights from electron localization function. Interdisciplinary Sciences, Computational Life Sciences, 2009, 1, 55-60.	2.2	13
110	Interactions within the alcohol dehydrogenase Zn(II)â€metalloenzyme active site: Interplay between subvalence, electron correlation/dispersion, and charge transfer/induction effects. International Journal of Quantum Chemistry, 2011, 111, 1213-1221.	1.0	13
111	Preface: Special Topic: From Quantum Mechanics to Force Fields. Journal of Chemical Physics, 2017, 147, 161401.	1.2	13
112	Interfacial Water Many-Body Effects Drive Structural Dynamics and Allosteric Interactions in SARS-CoV-2 Main Protease Dimerization Interface. Journal of Physical Chemistry Letters, 2021, 12, 6218-6226.	2.1	13
113	Study of the docking of competitive inhibitors at a model of tyrosinase active site: Insights from joint broken-symmetry/spin-flip DFT computations and ELF topological analysis. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 3-11.	2.2	12
114	Quantumâ€chemistry based calibration of the alkali metal cation series (Li⁺ï£¿Cs⁺) for largeâ€scale polarizable molecular mechanics/dynamics simulations. Journal of Computational Chemistry, 2015, 36, 285-302.	1.5	12
115	Solvation effects drive the selectivity in Dielsâ€“Alder reaction under hyperbaric conditions. Chemical Communications, 2020, 56, 6632-6635.	2.2	12
116	O(N) Stochastic Evaluation of Many-Body van der Waals Energies in Large Complex Systems. Journal of Chemical Theory and Computation, 2022, 18, 1633-1645.	2.3	12
117	Accurate Deep Learning-Aided Density-Free Strategy for Many-Body Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 4381-4388.	2.1	12
118	Development of the Quantum-Inspired SIBFA Many-Body Polarizable Force Field: Enabling Condensed-Phase Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, 18, 3607-3621.	2.3	12
119	Dioxygen Activation by Mononuclear Copper Enzymes: Insights from a Tripodal Ligand Mimicking Their CuM Coordination Sphere. Inorganic Chemistry, 2009, 48, 7003-7005.	1.9	11
120	Editorial: Special issue on quantum mechanical modeling of biological systems. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 1-2.	2.2	11
121	Unraveling Lowâ€Barrier Hydrogen Bonds in Complex Systems with a Simple Quantum Topological Criterion. Chemistry - A European Journal, 2011, 17, 2833-2837.	1.7	11
122	Complexes of a Znâ€metalloenzyme binding site with hydroxamateâ€containing ligands. A case for detailed benchmarkings of polarizable molecular mechanics/dynamics potentials when the experimental binding structure is unknown. Journal of Computational Chemistry, 2016, 37, 2770-2782.	1.5	11
123	Calibration of 1,2,4-Triazole-3-Thione, an Original Zn-Binding Group of Metallo-Î²-Lactamase Inhibitors. Validation of a Polarizable MM/MD Potential by Quantum Chemistry. Journal of Physical Chemistry B, 2017, 121, 6295-6312.	1.2	11
124	Importance of explicit smeared lone-pairs in anisotropic polarizable molecular mechanics. Torture track angular tests for exchange-repulsion and charge transfer contributions. Journal of Computational Chemistry, 2017, 38, 1897-1920.	1.5	11
125	Further refinements of next-generation force fields â€" Nonempirical localization of off-centered points in molecules. Canadian Journal of Chemistry, 2013, 91, 804-810.	0.6	10
126	Bridging organometallics and quantum chemical topology: Understanding electronic relocalisation during palladiumâ€catalyzed reductive elimination. Journal of Computational Chemistry, 2015, 36, 1167-1175.	1.5	10

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127	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. Journal of Chemical Theory and Computation, 2021, 17, 2323-2341.	2.3	10
128	Lead Substitution in Synaptotagmin: A Case Study. Journal of Physical Chemistry B, 2010, 114, 4005-4009.	1.2	9
129	From quantum mechanics to force fields: new methodologies for the classical simulation of complex systems. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	9
130	Polarizable molecular mechanics studies of <scp>Cu(I)/Zn(II)</scp> superoxide dismutase: Bimetallic binding site and structured waters. Journal of Computational Chemistry, 2014, 35, 2096-2106.	1.5	9
131	A coherent derivation of the Ewald summation for arbitrary orders of multipoles: The self-terms. Journal of Chemical Physics, 2018, 149, 124103.	1.2	9
132	Molecular Dynamics Using Nonvariational Polarizable Force Fields: Theory, Periodic Boundary Conditions Implementation, and Application to the Bond Capacity Model. Journal of Chemical Theory and Computation, 2019, 15, 6213-6224.	2.3	9
133	Understanding the Chemistry of Lead at a Molecular Level: The Pb(II) 6s6p Lone Pair Can Be Bisdirected in Proteins. Journal of Chemical Theory and Computation, 2013, 9, 2416-2424.	2.3	8
134	A Simple Isomerization of the Purine Scaffold of a Kinase Inhibitor, Roscovitine, Affords a Four- to Seven-Fold Enhancement of Its Affinity for Four CDKs. Could This Be Traced Back to Conjugation-Induced Stiffenings/Loosenings of Rotational Barriers?. ACS Omega, 2017, 2, 3467-3474.	1.6	8
135	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	8
136	Progress Towards Accurate Molecular Modeling of Metal Complexes Using Polarizable Force Fields. , 2009, , .		7
137	Competitive ligand/chelate binding in [Cu(TMPA)]+ and [Cu(tren)]+ based complexes. Catalysis Today, 2011, 177, 79-86.	2.2	7
138	Conformational analysis of a polyconjugated protein-binding ligand by joint quantum chemistry and polarizable molecular mechanics. Addressing the issues of anisotropy, conjugation, polarization, and multipole transferability. Journal of Molecular Modeling, 2014, 20, 2472.	0.8	7
139	Revisiting H₂O Nucleation around Au⁺ and Hg²⁺: The Peculiar â€œPseudo-Softâ€•Character of the Gold Cation. Journal of Chemical Theory and Computation, 2014, 10, 1900-1909.	2.3	7
140	Butanethiol adsorption and dissociation on Ag (111): A periodic DFT study. Surface Science, 2016, 646, 247-252.	0.8	7
141	Velocity jump processes: An alternative to multi-timestep methods for faster and accurate molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 024101.	1.2	7
142	An Efficient Gaussian-Accelerated Molecular Dynamics (GaMD) Multilevel Enhanced Sampling Strategy: Application to Polarizable Force Fields Simulations of Large Biological Systems. Journal of Chemical Theory and Computation, 2022, 18, 968-977.	2.3	6
143	Efficient and Accurate Description of Dielsâ€Alder Reactions Using Density Functional Theory**. ChemPhysChem, 2022, 23, .	1.0	6
144	Importance of backdonation in [Mâ€“(CO)]p+ complexes isoelectronic to [Auâ€“(CO)]+. Journal of Chemical Physics, 2010, 133, 124310.	1.2	5

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145	AMOEBA Polarizable Force Field Parameters of the Heme Cofactor in Its Ferrous and Ferric Forms. Journal of Chemical Theory and Computation, 2018, 14, 2705-2720.	2.3	5
146	Understanding the structure and electronic properties of Th⁴⁺-water complexes. Canadian Journal of Chemistry, 2013, 91, 821-831.	0.6	4
147	Multipolar Force Fields for Atomistic Simulations. , 2016, , 251-286.		4
148	The inhibition process of HIV-1 integrase by diketoacids molecules: Understanding the factors governing the better efficiency of dolutegravir. Biochemical and Biophysical Research Communications, 2017, 488, 433-438.	1.0	4
149	Calibration of the dianionic phosphate group: Validation on the recognition site of the homodimeric enzyme phosphoglucose isomerase. Journal of Computational Chemistry, 2020, 41, 839-854.	1.5	4
150	Reconciling NMR Structures of the HIV-1 Nucleocapsid Protein NCp7 Using Extensive Polarizable Force Field Free-Energy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 2013-2020.	2.3	4
151	Towards scalable and accurate molecular dynamics using the SIBFA polarizable force field. AIP Conference Proceedings, 2017, , .	0.3	3
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