Jean-Philip Piquemal

List of Publications by Year in Descending Order

154 papers	8,108 citations	45 h-index	86 g-index
190 ext. papers	9,543 ext. citations	5.3 avg, IF	6.22 L-index

#	Paper	IF	Citations
154	Computationally driven discovery of SARS-CoV-2 M inhibitors: from design to experimental validation.. *Chemical Science*, **2022**, 13, 3674-3687	9.4	2
153	Stochastic Evaluation of Many-Body van der Waals Energies in Large Complex Systems.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	4
152	Accurate Deep Learning-Aided Density-Free Strategy for Many-Body Dispersion-Corrected Density Functional Theory.. *Journal of Physical Chemistry Letters*, **2022**, 13, 4381-4388	6.4	1
151	Development of the Quantum-Inspired SIBFA Many-Body Polarizable Force Field: Enabling Condensed-Phase Molecular Dynamics Simulations.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	4
150	Improvement of the Gaussian Electrostatic Model by separate fitting of Coulomb and exchange-repulsion densities and implementation of a new dispersion term. *Journal of Chemical Physics*, **2021**, 155, 194103	3.9	1
149	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
148	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. *Journal of Chemical Theory and Computation*, **2021**, 17, 2323-2341	6.4	5
147	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	6.4	9
146	Atomistic Polarizable Embeddings: Energy, Dynamics, Spectroscopy, and Reactivity. *Accounts of Chemical Research*, **2021**, 54, 2812-2822	24.3	4
145	NCIPLOT and the analysis of noncovalent interactions using the reduced density gradient. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1497	7.9	18
144	High-resolution mining of the SARS-CoV-2 main protease conformational space: supercomputer-driven unsupervised adaptive sampling. *Chemical Science*, **2021**, 12, 4889-4907	9.4	17
143	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	6.4	2
142	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	6.4	7
141	NCIPLOT4: Fast, Robust, and Quantitative Analysis of Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2020**, 16, 4150-4158	6.4	57
140	Quantum-Chemistry Based Design of Halobenzene Derivatives With Augmented Affinities for the HIV-1 Viral G/C Base-Pair. *Frontiers in Chemistry*, **2020**, 8, 440	5	1
139	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	6.4	3
138	New Way for Probing Bond Strength. *Journal of Physical Chemistry A*, **2020**, 124, 1850-1860	2.8	43

137	Solvation effects drive the selectivity in Diels-Alder reaction under hyperbaric conditions. *Chemical Communications*, **2020**, 56, 6632-6635	5.8	3
136	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	3.5	3
135	Implementation of Geometry-Dependent Charge Flux into the Polarizable AMOEBA+ Potential. *Journal of Physical Chemistry Letters*, **2020**, 11, 419-426	6.4	23
134	Velocity jump processes: An alternative to multi-timestep methods for faster and accurate molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 024101	3.9	4
133	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	6.4	7
132	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. *Chemical Science*, **2019**, 10, 7200-7211	9.4	30
131	AMOEBA+ Classical Potential for Modeling Molecular Interactions. *Journal of Chemical Theory and Computation*, **2019**, 15, 4122-4139	6.4	53
130	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. *Chemical Reviews*, **2019**, 119, 7940-7995	68.1	206
129	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	6.4	12
128	Pushing the Limits of Multiple-Time-Step Strategies for Polarizable Point Dipole Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 2593-2599	6.4	16
127	Polarizable Force Fields for Biomolecular Simulations: Recent Advances and Applications. *Annual Review of Biophysics*, **2019**, 48, 371-394	21.1	152
126	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	7
125	Accurate Biomolecular Simulations Account for Electronic Polarization. *Frontiers in Molecular Biosciences*, **2019**, 6, 143	5.6	29
124	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	6.4	4
123	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. *Journal of Chemical Theory and Computation*, **2018**, 14, 2084-2108	6.4	122
122	The Independent Gradient Model: A New Approach for Probing Strong and Weak Interactions in Molecules from Wave Function Calculations. *ChemPhysChem*, **2018**, 19, 724-735	3.2	124
121	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
120	A coherent derivation of the Ewald summation for arbitrary orders of multipoles: The self-terms. *Journal of Chemical Physics*, **2018**, 149, 124103	3.9	5

119	Tinker 8: Software Tools for Molecular Design. *Journal of Chemical Theory and Computation*, **2018**, 14, 5273-5289	6.4	188
118	Elucidating the Phosphate Binding Mode of Phosphate-Binding Protein: The Critical Effect of Buffer Solution. *Journal of Physical Chemistry B*, **2018**, 122, 6371-6376	3.4	14
117	QM/MM Simulations with the Gaussian Electrostatic Model: A Density-based Polarizable Potential. *Journal of Physical Chemistry Letters*, **2018**, 9, 3062-3067	6.4	28
116	Capturing Many-Body Interactions with Classical Dipole Induction Models. *Journal of Chemical Theory and Computation*, **2017**, 13, 2751-2761	6.4	19
115	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	3.4	4
114	Calibration of 1,2,4-Triazole-3-Thione, an Original Zn-Binding Group of Metallo-β-Lactamase Inhibitors. Validation of a Polarizable MM/MD Potential by Quantum Chemistry. *Journal of Physical Chemistry B*, **2017**, 121, 6295-6312	3.4	11
113	Tinker-OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. *Journal of Computational Chemistry*, **2017**, 38, 2047-2055	3.5	70
112	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	3.4	18
111	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	3.9	15
110	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	3.5	11
109	Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2017**, 13, 4025-4033	6.4	61
108	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	3.9	6
107	Revealing strong interactions with the reduced density gradient: a benchmark for covalent, ionic and charge-shift bonds. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	45
106	Preface: Special Topic: From Quantum Mechanics to Force Fields. *Journal of Chemical Physics*, **2017**, 147, 161401	3.9	11
105	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
104	Towards scalable and accurate molecular dynamics using the SIBFA polarizable force field **2017**,		2
103	Butanethiol adsorption and dissociation on Ag (111): A periodic DFT study. *Surface Science*, **2016**, 646, 247-252	1.8	4
102	Multipolar Force Fields for Atomistic Simulations **2016**, 251-286		3

101	Complexes of a Zn-metalloenzyme binding site with hydroxamate-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	3.5	11
100	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
99	A QM/MM Approach Using the AMOEBA Polarizable Embedding: From Ground State Energies to Electronic Excitations. *Journal of Chemical Theory and Computation*, **2016**, 12, 3654-61	6.4	100
98	Interpretation of the reduced density gradient. *Molecular Physics*, **2016**, 114, 1406-1414	1.7	66
97	An optimized charge penetration model for use with the AMOEBA force field. *Physical Chemistry Chemical Physics*, **2016**, 19, 276-291	3.6	43
96	LICHEM: A QM/MM program for simulations with multipolar and polarizable force fields. *Journal of Computational Chemistry*, **2016**, 37, 1019-29	3.5	57
95	A Complete NCI Perspective: From New Bonds to Reactivity. *Challenges and Advances in Computational Chemistry and Physics*, **2016**, 491-527	0.7	11
94	Entasis through hook-and-loop fastening in a glycoligand with cumulative weak forces stabilizing Cu(I). *Journal of the American Chemical Society*, **2015**, 137, 1141-6	16.4	21
93	Could the "Janus-like" properties of the halobenzene CX bond (X=Cl, Br) be leveraged to enhance molecular recognition?. *Journal of Computational Chemistry*, **2015**, 36, 210-21	3.5	12
92	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, 9477-95	3.4	17
91	Bridging organometallics and quantum chemical topology: Understanding electronic relocalisation during palladium-catalyzed reductive elimination. *Journal of Computational Chemistry*, **2015**, 36, 1167-75	3.5	10
90	Quantum-chemistry based calibration of the alkali metal cation series (Li(+)-Cs(+)) for large-scale polarizable molecular mechanics/dynamics simulations. *Journal of Computational Chemistry*, **2015**, 36, 285-302	3.5	11
89	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, 2589-99	6.4	37
88	Approaching the double-faceted nature of the CX bond in halobenzenes with a bifunctional probe. *Chemical Physics Letters*, **2015**, 637, 51-57	2.5	2
87	Polarizable Force Fields for Biomolecular Modeling. *Reviews in Computational Chemistry*, **2015**, 51-86		29
86	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
85	Polarizable molecular dynamics in a polarizable continuum solvent. *Journal of Chemical Theory and Computation*, **2015**, 11, 623-34	6.4	37
84	Addressing the Issues of Non-isotropy and Non-additivity in the Development of Quantum Chemistry-Grounded Polarizable Molecular Mechanics. *Challenges and Advances in Computational Chemistry and Physics*, **2015**, 1-49	0.7	1

83	Unraveling non-covalent interactions within flexible biomolecules: from electron density topology to gas phase spectroscopy. *Physical Chemistry Chemical Physics*, **2014**, 16, 9876-91	3.6	124
82	Synthesis and structure-activity relationship of non-peptidic antagonists of neuropilin-1 receptor. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 4254-9	2.9	25
81	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	2	27
80	Revisiting HO Nucleation around Au and Hg: The Peculiar "Pseudo-Soft" Character of the Gold Cation. *Journal of Chemical Theory and Computation*, **2014**, 10, 1900-1909	6.4	6
79	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II.Towards Massively Parallel Computations using Smooth Particle Mesh Ewald. *Journal of Chemical Theory and Computation*, **2014**, 10, 1638-1651	6.4	66
78	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, 9772-82	2.8	14
77	DFT-steric-based energy decomposition analysis of intermolecular interactions. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	33
76	GEM*: A Molecular Electronic Density-Based Force Field for Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 1361-5	6.4	57
75	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, 7598-612	2.8	22
74	Characterizing Molecular Interactions in Chemical Systems. *IEEE Transactions on Visualization and Computer Graphics*, **2014**, 20, 2476-85	4	41
73	Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 953-8	6.4	28
72	Modeling organochlorine compounds and the □hole effect using a polarizable multipole force field. *Journal of Physical Chemistry B*, **2014**, 118, 6456-65	3.4	65
71	Quantum, classical, and hybrid QM/MM calculations in solution: general implementation of the ddCOSMO linear scaling strategy. *Journal of Chemical Physics*, **2014**, 141, 184108	3.9	37
70	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	2	7
69	A supervised fitting approach to force field parametrization with application to the SIBFA polarizable force field. *Journal of Computational Chemistry*, **2014**, 35, 1577-91	3.5	21
68	Polarizable molecular mechanics studies of Cu(I)/Zn(II) superoxide dismutase: bimetallic binding site and structured waters. *Journal of Computational Chemistry*, **2014**, 35, 2096-106	3.5	9
67	Are Bond Critical Points Really Critical for Hydrogen Bonding?. *Journal of Chemical Theory and Computation*, **2013**, 9, 3263-6	6.4	348
66	Understanding the structure and electronic properties of Th4+-water complexes. *Canadian Journal of Chemistry*, **2013**, 91, 821-831	0.9	4

65	Towards energy decomposition analysis for open and closed shell f-elements mono aqua complexes. *Chemical Physics Letters*, **2013**, 563, 25-29	2.5	16
64	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, 2416-24	6.4	7
63	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, 2156-60	6.4	42
62	Could an anisotropic molecular mechanics/dynamics potential account for sigma hole effects in the complexes of halogenated compounds?. *Journal of Computational Chemistry*, **2013**, 34, 1125-35	3.5	20
61	Further refinements of next-generation force fields Nonempirical localization of off-centered points in molecules. *Canadian Journal of Chemistry*, **2013**, 91, 804-810	0.9	10
60	Toward a ligand specific of Pb2+ with respect to the Zn2+ and Ca2+ cations: A track from quantum chemistry. *Chemical Physics Letters*, **2012**, 532, 9-12	2.5	2
59	Coupling quantum interpretative techniques: another look at chemical mechanisms in organic reactions. *Journal of Chemical Theory and Computation*, **2012**, 8, 3993-3997	6.4	90
58	Ionic interactions: Comparative topological approach. *Computational and Theoretical Chemistry*, **2012**, 998, 193-201	2	31
57	Modeling Structural Coordination and Ligand Binding in Zinc Proteins with a Polarizable Potential. *Journal of Chemical Theory and Computation*, **2012**, 8, 1314-1324	6.4	88
56	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	1.9	51
55	Electron Pair Localization Function (EPLF) for Density Functional Theory and ab Initio Wave Function-Based Methods: A New Tool for Chemical Interpretation. *Journal of Chemical Theory and Computation*, **2011**, 7, 618-24	6.4	17
54	Correlation between electron localization and metal ion mutagenicity in DNA synthesis from QM/MM calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 11239-47	3.6	18
53	NCIPLOT: a program for plotting non-covalent interaction regions. *Journal of Chemical Theory and Computation*, **2011**, 7, 625-632	6.4	2067
52	Competitive ligand/chelate binding in [Cu(TMPA)]+ and [Cu(tren)]+ based complexes. *Catalysis Today*, **2011**, 177, 79-86	5.3	6
51	Enforcing hemidirectionality in Pb(II) complexes: The importance of anionic ligands. *Chemical Physics Letters*, **2011**, 510, 27-30	2.5	14
50	The reaction mechanism of type I phosphomannose isomerases: new information from inhibition and polarizable molecular mechanics studies. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 203-20	4.2	21
49	Interactions within the alcohol dehydrogenase Zn(II)-metalloenzyme active site: Interplay between subvalence, electron correlation/dispersion, and charge transfer/induction effects. *International Journal of Quantum Chemistry*, **2011**, 111, 1213-1221	2.1	13
48	Spin-driven activation of dioxygen in various metalloenzymes and their inspired models. *Journal of Computational Chemistry*, **2011**, 32, 1178-82	3.5	13

47	Many-body exchange-repulsion in polarizable molecular mechanics. I. Orbital-based approximations and applications to hydrated metal cation complexes. *Journal of Computational Chemistry*, **2011**, 32, 2949-57	3.5	30
46	Unraveling low-barrier hydrogen bonds in complex systems with a simple quantum topological criterion. *Chemistry - A European Journal*, **2011**, 17, 2833-7	4.8	10
45	Role of Cation Polarization in holo- and hemi-Directed [Pb(H2O)n](2+) Complexes and Development of a Pb(2+) Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2011**, 7, 138-47	6.4	19
44	Polarizable water networks in ligand-metalloprotein recognition. Impact on the relative complexation energies of Zn-dependent phosphomannose isomerase with D-mannose 6-phosphate surrogates. *Journal of Physical Chemistry B*, **2011**, 115, 8304-16	3.4	30
43	Importance of backdonation in [M-(CO)]p+ complexes isoelectronic to [Au-(CO)]+. *Journal of Chemical Physics*, **2010**, 133, 124310	3.9	4
42	Understanding selectivity of hard and soft metal cations within biological systems using the subvalence concept. I. Application to blood coagulation: direct cation-protein electronic effects vs. indirect interactions through water networks. *Journal of Chemical Theory and Computation*, **2010**, 6, 1048-1063	6.4	51
41	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, 11860-3	16.4	80
40	Analysis of the interactions taking place in the recognition site of a bimetallic Mg(II)-Zn(II) enzyme, isopentenyl diphosphate isomerase. a parallel quantum-chemical and polarizable molecular mechanics study. *Journal of Physical Chemistry B*, **2010**, 114, 4884-95	3.4	18
39	Lead substitution in synaptotagmin: a case study. *Journal of Physical Chemistry B*, **2010**, 114, 4005-9	3.4	8
38	Polarizable water molecules in ligand-macromolecule recognition. Impact on the relative affinities of competing pyrrolopyrimidine inhibitors for FAK kinase. *Journal of the American Chemical Society*, **2010**, 132, 3312-20	16.4	48
37	Polarizable molecular dynamics simulation of Zn(II) in water using the AMOEBA force field. *Journal of Chemical Theory and Computation*, **2010**, 6, 2059-2070	6.4	124
36	Gaussian Multipole Model (GMM). *Journal of Chemical Theory and Computation*, **2010**, 6, 190-202	6.4	68
35	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	3.5	10
34	Progress Towards Accurate Molecular Modeling of Metal Complexes Using Polarizable Force Fields **2009**,		5
33	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	3.5	13
32	Beyond holo/hemidirectionality in Pb(II) complexes: Can the valence lone pair be bisdirected?. *Chemical Physics Letters*, **2009**, 478, 17-19	2.5	14
31	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, 7100-7	3.4	19
30	Dioxygen activation by mononuclear copper enzymes: insights from a tripodal ligand mimicking their Cu(M) coordination sphere. *Inorganic Chemistry*, **2009**, 48, 7003-5	5.1	11

29	New intermolecular benchmark calculations on the water dimer: SAPT and supermolecular post-Hartree□ock approaches. *International Journal of Quantum Chemistry*, **2009**, 109, 3259-3267	2.1	24
28	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	0.7	17
27	Fragment-Localized Kohn-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, 2020-9	6.4	47
26	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, 1659-68	6.4	21
25	Simple Formulas for Improved Point-Charge Electrostatics in Classical Force Fields and Hybrid Quantum Mechanical/Molecular Mechanical Embedding. *International Journal of Quantum Chemistry*, **2008**, 108, 1905-1912	2.1	51
24	Understanding lead chemistry from topological insights: the transition between holo- and hemidirected structures within the [Pb(CO)n]2+ model series. *Chemistry - A European Journal*, **2008**, 14, 2730-43	4.8	36
23	Advancing beyond charge analysis using the electronic localization function: Chemically intuitive distribution of electrostatic moments. *Journal of Computational Chemistry*, **2008**, 29, 1440-9	3.5	56
22	Key role of the polarization anisotropy of water in modeling classical polarizable force fields. *Journal of Physical Chemistry A*, **2007**, 111, 8170-6	2.8	70
21	Toward a Separate Reproduction of the Contributions to the Hartree-Fock and DFT Intermolecular Interaction Energies by Polarizable Molecular Mechanics with the SIBFA Potential. *Journal of Chemical Theory and Computation*, **2007**, 3, 824-37	6.4	93
20	Specificity of acyl transfer from 2-mercaptobenzamide thioesters to the HIV-1 nucleocapsid protein. *Journal of the American Chemical Society*, **2007**, 129, 11067-78	16.4	50
19	Anisotropic, Polarizable Molecular Mechanics Studies of Inter- and Intramolecular Interactions and Ligand-Macromolecule Complexes. A Bottom-Up Strategy. *Journal of Chemical Theory and Computation*, **2007**, 3, 1960-1986	6.4	281
18	Binding of 5-phospho-D-arabinonohydroxamate and 5-phospho-D-arabinonate inhibitors to zinc phosphomannose isomerase from Candida albicans studied by polarizable molecular mechanics and quantum mechanics. *Journal of Computational Chemistry*, **2007**, 28, 938-57	3.5	40
17	Numerical fitting of molecular properties to Hermite Gaussians. *Journal of Physical Chemistry A*, **2007**, 111, 12049-56	2.8	28
16	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 (M(p+) = Cu+, Zn2+, Ag+, Cd2+, Au+, Hg2+). *Journal of Computational Chemistry*, **2006**, 27, 142-56	3.5	37
15	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	3.9	163
14	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	3.9	91
13	[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	3.9	29
12	Towards a force field based on density fitting. *Journal of Chemical Physics*, **2006**, 124, 104101	3.9	162

11	Quantum mechanics/molecular mechanics electrostatic embedding with continuous and discrete functions. *Journal of Physical Chemistry B*, **2006**, 110, 13682-4	3.4	48
10	Comments on the nature of the bonding in oxygenated dinuclear copper enzyme models. *Computational and Theoretical Chemistry*, **2006**, 764, 77-86		18
9	Intermolecular electrostatic energies using density fitting. *Journal of Chemical Physics*, **2005**, 123, 044109	3.9	52
8	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, 1052-62	3.5	95
7	Representation of Zn(II) complexes in polarizable molecular mechanics. Further refinements of the electrostatic and short-range contributions. Comparisons with parallel ab initio computations. *Journal of Computational Chemistry*, **2005**, 26, 1113-30	3.5	73
6	Complexes of thiomandelate and captopril mercaptocarboxylate inhibitors to metallo-beta-lactamase by polarizable molecular mechanics. Validation on model binding sites by quantum chemistry. *Journal of Computational Chemistry*, **2005**, 26, 1131-47	3.5	47
5	Inclusion of the ligand field contribution in a polarizable molecular mechanics: SIBFA-LF. *Journal of Computational Chemistry*, **2004**, 25, 308-308	3.5	
4	Inclusion of the ligand field contribution in a polarizable molecular mechanics: SIBFA-LF. *Journal of Computational Chemistry*, **2003**, 24, 1963-70	3.5	64
3	Theoretical study of phenol and 2-aminophenol docking at a model of the tyrosinase active site. *New Journal of Chemistry*, **2003**, 27, 909	3.6	12
2	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, 10353-9	2.8	128
1	Spectrometric and computational studies of the binding of HIV-1 integrase inhibitors to viral DNA extremities1, e6		1