

# George A Kaminski

## List of Publications by Year in descending order

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30  
papers

5,605  
citations

394286

19  
h-index

477173

29  
g-index

30  
all docs

30  
docs citations

30  
times ranked

6988  
citing authors

#	ARTICLE	IF	CITATIONS
1	Evaluation and Reparametrization of the OPLS-AA Force Field for Proteins via Comparison with Accurate Quantum Chemical Calculations on Peptides. <i>Journal of Physical Chemistry B</i> , 2001, 105, 6474-6487.	1.2	3,513
2	Free Energies of Hydration and Pure Liquid Properties of Hydrocarbons from the OPLS All-Atom Model. <i>The Journal of Physical Chemistry</i> , 1994, 98, 13077-13082.	2.9	300
3	Development of a polarizable force field for proteins via ab initio quantum chemistry: First generation model and gas phase tests. <i>Journal of Computational Chemistry</i> , 2002, 23, 1515-1531.	1.5	296
4	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. <i>Journal of Chemical Physics</i> , 1999, 110, 741-754.	1.2	251
5	Performance of the AMBER94, MMFF94, and OPLS-AA Force Fields for Modeling Organic Liquids. <i>The Journal of Physical Chemistry</i> , 1996, 100, 18010-18013.	2.9	242
6	Development of an Accurate and Robust Polarizable Molecular Mechanics Force Field from ab Initio Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2004, 108, 621-627.	1.1	221
7	Force Field Validation Using Protein Side Chain Prediction. <i>Journal of Physical Chemistry B</i> , 2002, 106, 11673-11680.	1.2	165
8	A Quantum Mechanical and Molecular Mechanical Method Based on CM1A Charges: Applications to Solvent Effects on Organic Equilibria and Reactions. <i>Journal of Physical Chemistry B</i> , 1998, 102, 1787-1796.	1.2	113
9	A Polarizable Force Field and Continuum Solvation Methodology for Modeling of Protein-Ligand Interactions. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 694-715.	2.3	100
10	A computationally inexpensive modification of the point dipole electrostatic polarization model for molecular simulations. <i>Journal of Computational Chemistry</i> , 2003, 24, 267-276.	1.5	56
11	Accurate Prediction of Absolute Acidity Constants in Water with a Polarizable Force Field: Substituted Phenols, Methanol, and Imidazole. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5884-5890.	1.2	48
12	Electrostatic Polarization Is Crucial for Reproducing pKa Shifts of Carboxylic Residues in Turkey Ovomucoid Third Domain. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9036-9044.	1.2	34
13	Pseudospectral Local Second-Order Møller-Plesset Methods for Computation of Hydrogen Bonding Energies of Molecular Pairs. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 248-254.	2.3	32
14	Quality of random number generators significantly affects results of Monte Carlo simulations for organic and biological systems. <i>Journal of Computational Chemistry</i> , 2011, 32, 513-524.	1.5	31
15	Binding of Copper and Cisplatin to Atx1 Is Mediated by Glutathione through the Formation of Metal-Sulfur Clusters. <i>Biochemistry</i> , 2017, 56, 3129-3141.	1.2	27
16	Polarizable Simulations with Second-Order Interaction Model Force Field and Software for Fast Polarizable Calculations: Parameters for Small Model Systems and Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2935-2943.	2.3	26
17	Calculating $pK_a$ values for substituted phenols and hydration energies for other compounds with the first-order fuzzy continuum solvation model. <i>Journal of Computational Chemistry</i> , 2012, 33, 2388-2399.	1.5	23
18	Reproducing Basic $pK_a$ Values for Turkey Ovomucoid Third Domain Using a Polarizable Force Field. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7844-7850.	1.2	20

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19	Polarizable Simulations with Second-Order Interaction Model (POSSIM) Force Field: Developing Parameters for Alanine Peptides and Protein Backbone. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1415-1427.	2.3	19
20	PKA17: A Coarse-Grain Grid-Based Methodology and Web-Based Software for Predicting Protein pK <sub>a</sub> Shifts. <i>Journal of Computational Chemistry</i> , 2019, 40, 1718-1726.	1.5	17
21	Electrostatic Polarization Is Crucial in Reproducing Cu(I) Interaction Energies and Hydration. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10079-10085.	1.2	15
22	Importance of electrostatic polarizability in calculating cysteine acidity constants and copper(I) binding energy of <i>Bacillus subtilis</i> CopZ. <i>Journal of Computational Chemistry</i> , 2012, 33, 1142-1151.	1.5	15
23	Polarizable simulations with second order interaction model (POSSIM) force field: Developing parameters for protein side-chain analogues. <i>Journal of Computational Chemistry</i> , 2013, 34, 1241-1250.	1.5	10
24	POSSIM: Parameterizing Complete Second-Order Polarizable Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4896-4910.	2.3	10
25	Effects of Lysine Substitution on Stability of Polyalanine $\alpha$ Helix. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4691-4706.	2.3	8
26	Developing multisite empirical force field models for Pt(II) and cisplatin. <i>Journal of Computational Chemistry</i> , 2017, 38, 161-168.	1.5	5
27	Computational Studies of the Effect of Shock Waves on the Binding of Model Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4972-4981.	2.3	3
28	Using polarizable POSSIM force field and fuzzy-border continuum solvent model to calculate pK <sub>a</sub> shifts of protein residues. <i>Journal of Computational Chemistry</i> , 2017, 38, 65-80.	1.5	3
29	Expansion and Additional Validation of PKA17: A Fast Real-Time and Web-Based pKa Predictor. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 141-152.	1.0	2
30	Expansion and additional validation of PKA17: A fast real-time and web-based pKa predictor. <i>Journal of Theoretical and Computational Chemistry</i> , 0, , 2042003.	1.8	0