Thomas Fox

List of Publications by Year in Descending Order

50 papers	14,179 citations	29 h-index	50 g-index
50 ext. papers	15,026 ext. citations	6.6 avg, IF	5.6 L-index

#	Paper	IF	Citations
50	Protein-ligand free energies of binding from full-protein DFT calculations: convergence and choice of exchange-correlation functional. *Physical Chemistry Chemical Physics*, **2021**, 23, 9381-9393	3.6	9
49	Assessing the accuracy of octanol-water partition coefficient predictions in the SAMPL6 Part II log□P Challenge. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 335-370	4.2	29
48	Peptidic Macrocycles - Conformational Sampling and Thermodynamic Characterization. *Journal of Chemical Information and Modeling*, **2018**, 58, 982-992	6.1	38
47	Intuitive Density Functional Theory-Based Energy Decomposition Analysis for Protein-Ligand Interactions. *Journal of Chemical Theory and Computation*, **2017**, 13, 1837-1850	6.4	14
46	Energy Decomposition Analysis Based on Absolutely Localized Molecular Orbitals for Large-Scale Density Functional Theory Calculations in Drug Design. *Journal of Chemical Theory and Computation* , **2016**, 12, 3135-48	6.4	14
45	A "Stepping Stone" Approach for Obtaining Quantum Free Energies of Hydration. *Journal of Physical Chemistry B*, **2015**, 119, 7030-40	3.4	32
44	Energy decomposition analysis approaches and their evaluation on prototypical protein-drug interaction patterns. *Chemical Society Reviews*, **2015**, 44, 3177-211	58.5	204
43	Heteroaromatic □stacking energy landscapes. *Journal of Chemical Information and Modeling*, **2014**, 54, 1371-9	6.1	113
42	Accuracy assessment and automation of free energy calculations for drug design. *Journal of Chemical Information and Modeling*, **2014**, 54, 108-20	6.1	99
41	Density functional theory calculations on entire proteins for free energies of binding: application to a model polar binding site. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 3335-46	4.2	28
40	Large-scale DFT calculations in implicit solvent□A case study on the T4 lysozyme L99A/M102Q protein. *International Journal of Quantum Chemistry*, **2013**, 113, 771-785	2.1	29
39	Free energies of binding from large-scale first-principles quantum mechanical calculations: application to ligand hydration energies. *Journal of Physical Chemistry B*, **2013**, 117, 9478-85	3.4	39
38	Economical and accurate protocol for calculating hydrogen-bond-acceptor strengths. *Journal of Chemical Information and Modeling*, **2013**, 53, 3262-72	6.1	14
37	A GRID-derived water network stabilizes molecular dynamics computer simulations of a protease. *Journal of Chemical Information and Modeling*, **2011**, 51, 2860-7	6.1	13
36	Protein and metal cluster structure of the wheat metallothionein domain □E(c)-1: the second part of the puzzle. *Journal of Biological Inorganic Chemistry*, **2011**, 16, 683-94	3.7	44
35	A challenging system: free energy prediction for factor Xa. *Journal of Computational Chemistry*, **2011**, 32, 1743-52	3.5	55
34	First Principles-Based Calculations of Free Energy of Binding: Application to Ligand Binding in a Self-Assembling Superstructure. *Journal of Chemical Theory and Computation*, **2011**, 7, 1102-8	6.4	17

33	Electrostatic embedding in large-scale first principles quantum mechanical calculations on biomolecules. *Journal of Chemical Physics*, **2011**, 135, 224107	3.9	44
32	Dispersion dominated halogen-π interactions: energies and locations of minima. *Physical Chemistry Chemical Physics*, **2010**, 12, 14941-9	3.6	69
31	Stabilizing of a globular protein by a highly complex water network: a molecular dynamics simulation study on factor Xa. *Journal of Physical Chemistry B*, **2010**, 114, 7405-12	3.4	49
30	Bias-correction of regression models: a case study on hERG inhibition. *Journal of Chemical Information and Modeling*, **2009**, 49, 1486-96	6.1	27
29	Computational approaches to predict drug metabolism. *Expert Opinion on Drug Metabolism and Toxicology*, **2009**, 5, 15-27	5.5	36
28	Chapter 5 Linear Quantitative Structure–Activity Relationships for the Interaction of Small Molecules with Human Cytochrome P450 Isoenzymes. *Annual Reports in Computational Chemistry*, **2007**, 63-81	1.8	2
27	Machine learning techniques for in silico modeling of drug metabolism. *Current Topics in Medicinal Chemistry*, **2006**, 6, 1579-91	3	75
26	Multivariate modeling of cytochrome P450 3A4 inhibition. *European Journal of Pharmaceutical Sciences*, **2005**, 24, 451-63	5.1	40
25	A support vector machine approach to classify human cytochrome P450 3A4 inhibitors. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 189-201	4.2	50
24	Prediction of Human Cytochrome P450 Inhibition Using Support Vector Machines. *QSAR and Combinatorial Science*, **2005**, 24, 491-502		33
23	Protein Selectivity Studies Using GRID-MIFs. *Methods and Principles in Medicinal Chemistry*, **2005**, 43-82	0.4	1
22	Onion design and its application to a pharmaceutical QSAR problem. *Journal of Chemometrics*, **2004**, 18, 188-202	1.6	25
21	Computer based screening of compound databases: 1. Preselection of benzamidine-based thrombin inhibitors. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 411-25	4.2	13
20	GRID/CPCA: a new computational tool to design selective ligands. *Journal of Medicinal Chemistry*, **2000**, 43, 3033-44	8.3	179
19	Use of Locally Enhanced Sampling in Free Energy Calculations: Testing and Application to the α↔β Anomerization of Glucose. *Journal of the American Chemical Society*, **1998**, 120, 5771-5782	16.4	85
18	Application of the RESP Methodology in the Parametrization of Organic Solvents. *Journal of Physical Chemistry B*, **1998**, 102, 8070-8079	3.4	421
17	A molecular level picture of the stabilization of A-DNA in mixed ethanol-water solutions. *Proceedings of the National Academy of Sciences of the United States of America*, **1997**, 94, 9626-30	11.5	99
16	Ligand Binding in the Catalytic Antibody 17E8. A Free Energy Perturbation Calculation Study. *Journal of the American Chemical Society*, **1997**, 119, 11571-11577	16.4	35

15	The development/application of a minimalist organic/biochemical molecular mechanic force field using a combination of ab initio calculations and experimental data **1997**, 83-96		156
14	Application of Free Energy Perturbation Calculations to the Tennis Ball Dimer: Why Is CF4 Not Encapsulated by This Host?. *The Journal of Physical Chemistry*, **1996**, 100, 10779-10783		15
13	Calculation of Ionization Potentials and CH Bond Dissociation Energies of Toluene Derivatives. *The Journal of Physical Chemistry*, **1996**, 100, 2950-2956		54
12	The application of different solvation and electrostatic models in molecular dynamics simulations of ubiquitin: how well is the X-ray structure "maintained"?. *Proteins: Structure, Function and Bioinformatics*, **1996**, 25, 315-34	4.2	80
11	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. *Journal of the American Chemical Society*, **1995**, 117, 5179-5197	16.4	10990
10	Calculation of Electronic Spectra of Hydrated Ln(III) Ions within the INDO/S-CI Approach. *The Journal of Physical Chemistry*, **1995**, 99, 600-605		14
9	Molecular Dynamics Simulations on Solvated Biomolecular Systems: The Particle Mesh Ewald Method Leads to Stable Trajectories of DNA, RNA, and Proteins. *Journal of the American Chemical Society*, **1995**, 117, 4193-4194	16.4	659
8	Design of rigid donor-acceptor systems with a low-lying charge-transfer state: an INDO model study of barrelene-based compounds. *The Journal of Physical Chemistry*, **1993**, 97, 11420-11426		7
7	Electrostatic solvent effects on the electronic structure of ground and excited states of molecules: Applications of a cavity model based upon a finite element method. *Journal of Computational Chemistry*, **1993**, 14, 253-262	3.5	32
6	On the electronic structure of barrelene-based rigid organic donor-acceptor systems. A comparison of INDO/S-CI calculations with absorption and fluorescence emission spectra. *Chemical Physics*, **1993**, 175, 357-367	2.3	1
5	On the electronic structure of barrelene-based rigid organic donor-acceptor systems. An INDO model study including solvent effects. *International Journal of Quantum Chemistry*, **1992**, 44, 551-561	2.1	2
4	On the cavity model for solvent shifts of excited states a critical appraisal. *Computational and Theoretical Chemistry*, **1992**, 276, 279-297		13
3	The calculation of solvatochromic shifts: the n- transition of acetone. *Chemical Physics Letters*, **1992**, 191, 33-37	2.5	61
2	Modeling of the geometry of densely packed chemisorbed overlayers: small organic molecules on Ni(110) and Pd(110). *Surface Science*, **1991**, 256, 159-170	1.8	19
1	Assessing the accuracy of octanol-water partition coefficient predictions in the SAMPL6 Part II logPChallenge		2