Ian Gould

List of Publications by Year in Descending Order

48 papers	13,243 citations	22 h-index	54 g-index
54 ext. papers	14,177 ext. citations	4.8 avg, IF	5.44 L-index

#	Paper	IF	Citations
48	Modulation of cardiac thin filament structure by phosphorylated troponin-I analyzed by protein-protein docking and molecular dynamics simulation.. *Archives of Biochemistry and Biophysics* , **2022**, 109282	4.1	2
47	Design, synthesis and evaluation of a tripodal receptor for phosphatidylinositol phosphates. *Scientific Reports*, **2020**, 10, 18450	4.9	0
46	A TDDFT investigation of the Photosystem II reaction center: Insights into the precursors to charge separation. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 19705-19712	11.5	4
45	A computational study of Anthracyclines interacting with lipid bilayers: Correlation of membrane insertion rates, orientation effects and localisation with cytotoxicity. *Scientific Reports*, **2019**, 9, 2155	4.9	9
44	Modeling the Effect of BSEP Inhibitors in Lipid Bilayers by Means of All-Atom Molecular Dynamics Simulation. *ACS Omega*, **2019**, 4, 3341-3350	3.9	2
43	Mechanism of Photoinduced Triplet Intermolecular Hydrogen Transfer between Cycloxydim and Chlorothalonil. *Journal of Physical Chemistry A*, **2018**, 122, 4285-4293	2.8	2
42	Troponin structure: its modulation by Ca(2+) and phosphorylation studied by molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 20691-707	3.6	14
41	Simulation of lipid bilayer self-assembly using all-atom lipid force fields. *Physical Chemistry Chemical Physics*, **2016**, 18, 10573-84	3.6	32
40	The Parasol Protocol for computational mutagenesis. *Protein Engineering, Design and Selection*, **2016**, 29, 253-61	1.9	2
39	Molecular dynamics studies on the DNA-binding process of ERG. *Molecular BioSystems*, **2016**, 12, 3600-3610		5
38	Imaging plasma membrane phase behaviour in live cells using a thiophene-based molecular rotor. *Chemical Communications*, **2016**, 52, 13269-13272	5.8	29
37	Imaging phase separation in model lipid membranes through the use of BODIPY based molecular rotors. *Physical Chemistry Chemical Physics*, **2015**, 17, 18393-402	3.6	66
36	A Parameterization of Cholesterol for Mixed Lipid Bilayer Simulation within the Amber Lipid14 Force Field. *Journal of Physical Chemistry B*, **2015**, 119, 12424-35	3.4	38
35	All-atom lipid bilayer self-assembly with the AMBER and CHARMM lipid force fields. *Chemical Communications*, **2015**, 51, 4402-5	5.8	40
34	Lipid14: The Amber Lipid Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 865-879	6.4	725
33	Understanding the relative affinity and specificity of the pleckstrin homology domain of protein kinase B for inositol phosphates. *Physical Chemistry Chemical Physics*, **2012**, 14, 929-36	3.6	13
32	Mutational Locally Enhanced Sampling (MULES) for quantitative prediction of the effects of mutations at protein–protein interfaces. *Chemical Science*, **2012**, 3, 1503	9.4	2

31	GAFFlipid: a General Amber Force Field for the accurate molecular dynamics simulation of phospholipid. *Soft Matter*, **2012**, 8, 9617	3.6	151
30	A theoretical investigation of inositol 1,3,4,5-tetrakisphosphate. *Physical Chemistry Chemical Physics* , **2011**, 13, 1070-81	3.6	7
29	Potential for the detection of molecular complexes and determination of interaction geometry by 2DIR: application to protein sciences. *Faraday Discussions*, **2011**, 150, 161-74; discussion 257-92	3.6	7
28	Comparing experimental and computational alanine scanning techniques for probing a prototypical protein-protein interaction. *Protein Engineering, Design and Selection*, **2011**, 24, 197-207	1.9	62
27	Further evaluation of quantum chemical methods for the prediction of non-specific binding of positron emission tomography tracers. *Physical Chemistry Chemical Physics*, **2011**, 13, 21552-7	3.6	7
26	Assessment of standard force field models against high-quality ab initio potential curves for prototypes of pi-pi, CH/pi, and SH/pi interactions. *Journal of Computational Chemistry*, **2009**, 30, 2187-93	3.5	81
25	Biological and biomedical applications of two-dimensional vibrational spectroscopy: proteomics, imaging, and structural analysis. *Accounts of Chemical Research*, **2009**, 42, 1322-31	24.3	44
24	Detection of complex formation and determination of intermolecular geometry through electrical anharmonic coupling of molecular vibrations using electron-vibration-vibration two-dimensional infrared spectroscopy. *Physical Chemistry Chemical Physics*, **2009**, 11, 8417-21	3.6	22
23	Protein identification and quantification by two-dimensional infrared spectroscopy: implications for an all-optical proteomic platform. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 15352-7	11.5	40
22	Structure and dynamics of phospholipid bilayers using recently developed general all-atom force fields. *Journal of Computational Chemistry*, **2008**, 29, 24-37	3.5	76
21	Ab initio computational study of positron emission tomography ligands interacting with lipid molecule for the prediction of nonspecific binding. *Journal of Computational Chemistry*, **2008**, 29, 2397-405	3.5	23
20	Optical fingerprinting of peptides using two-dimensional infrared spectroscopy: proof of principle. *Analytical Biochemistry*, **2008**, 374, 358-65	3.1	29
19	Decongestion of methylene spectra in biological and non-biological systems using picosecond 2DIR spectroscopy measuring electron-vibration□ibration coupling. *Chemical Physics*, **2008**, 350, 201-211	2.3	21
18	Comparison of basis set effects and the performance of ab initio and DFT methods for probing equilibrium fluctuations. *Journal of Computational Chemistry*, **2007**, 28, 478-90	3.5	19
17	Correlated ab initio quantum chemical calculations of di- and trisaccharide conformations. *Journal of Computational Chemistry*, **2007**, 28, 1965-73	3.5	10
16	The Effect of pH on the Photophysics and Photochemistry of Di-sulphonated Aluminum Phthalocyanine. *Photochemistry and Photobiology*, **2007**, 71, 397-404	3.6	3
15	Direct identification and decongestion of Fermi resonances by control of pulse time ordering in two-dimensional IR spectroscopy. *Journal of Chemical Physics*, **2007**, 127, 114513	3.9	30
14	The Structure of Imidazolium-Based Ionic Liquids: Insights From Ion-Pair Interactions. *Australian Journal of Chemistry*, **2007**, 60, 9	1.2	182

13	Structural characterization of the 1-butyl-3-methylimidazolium chloride ion pair using ab initio methods. *Journal of Physical Chemistry A*, **2006**, 110, 2269-82	2.8	184
12	Glyoxylate as a backbone linkage for a prebiotic ancestor of RNA. *Origins of Life and Evolution of Biospheres*, **2006**, 36, 39-63	1.5	62
11	Molecular dynamics simulations of LysRS: an asymmetric state. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 649-62	4.2	12
10	Effect of adiabaticity on electron dynamics in zinc myoglobin. *Journal of Physical Chemistry B*, **2005**, 109, 5954-61	3.4	6
9	A combined QM and MM investigation into guanine quadruplexes. *Journal of Molecular Graphics and Modelling*, **2005**, 24, 138-46	2.8	19
8	Functional asymmetry in the lysyl-tRNA synthetase explored by molecular dynamics, free energy calculations and experiment. *BMC Structural Biology*, **2003**, 3, 5	2.7	19
7	Large and Fast Relaxations inside a Protein: Calculation and Measurement of Reorganization Energies in Alcohol Dehydrogenase. *Journal of Physical Chemistry B*, **2002**, 106, 11658-11665	3.4	69
6	Computational Chemistry: Application to Biological Systems. *Molecular Simulation*, **2001**, 26, 73-83	2	3
5	Triplet 1-Nitronaphthalene and Competitive Energy and Electron Transfer Reactions With Trans-Stilbene. *Laser Chemistry*, **1999**, 19, 397-401		1
4	A Quantum Mechanical/Molecular Mechanical Approach to Relaxation Dynamics: Calculation of the Optical Properties of Solvated Bacteriochlorophyll-a. *Journal of Physical Chemistry B*, **1999**, 103, 7720-7727	3.4	54
3	A Quantum Mechanical/Molecular Mechanical Approach to Solvation Dynamics Tested by Three Pulse Photon Echo Measurements. *Springer Series in Chemical Physics*, **1998**, 532-534	0.3	2
2	Optical properties of solvated molecules calculated by a QMMM method Chlorophyll a and bacteriochlorophyll a. *Faraday Discussions*, **1997**, 108, 51-62	3.6	19
1	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