Robert W Gra

List of Publications by Year in Descending Order

68 papers	1,418 citations	22 h-index	34 g-index
73 ext. papers	1,563 ext. citations	4.5 avg, IF	4.46 L-index

#	Paper	IF	Citations
68	Ribose Alters the Photochemical Properties of the Nucleobase in Thionated Nucleosides. *Journal of Physical Chemistry Letters*, **2021**, 12, 6707-6713	6.4	1
67	Stereoselectivity Enhancement During the Generation of Three Contiguous Stereocenters in Tetrahydrothiophenes. *ChemCatChem*, **2021**, 13, 574-580	5.2	1
66	Ultrafast nonradiative deactivation of photoexcited 8-oxo-hypoxanthine: a nonadiabatic molecular dynamics study. *Physical Chemistry Chemical Physics*, **2021**, 23, 1234-1241	3.6	0
65	An effective potential for Frenkel excitons. *Physical Chemistry Chemical Physics*, **2021**, 23, 1923-1935	3.6	0
64	Ab initio effective one-electron potential operators: Applications for charge-transfer energy in effective fragment potentials. *Journal of Computational Chemistry*, **2021**, 42, 398-411	3.5	1
63	Selective prebiotic formation of RNA pyrimidine and DNA purine nucleosides. *Nature*, **2020**, 582, 60-66	50.4	52
62	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. II. Halogen-bonded systems. *Physical Chemistry Chemical Physics*, **2020**, 22, 4225-4234	3.6	2
61	UV-induced hydrogen transfer in DNA base pairs promoted by dark nπ^* states. *Chemical Communications*, **2019**, 56, 201-204	5.8	4
60	Applications of Thermal Activation, Ball-milling and Aqueous Medium in Stereoselective Michael Addition of Nitromethane to Enynones Catalyzed by Chiral Squaramides. *Advanced Synthesis and Catalysis*, **2019**, 361, 1108-1116	5.6	11
59	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. *Physical Chemistry Chemical Physics*, **2018**, 20, 19841-19849	3.6	9
58	Photostability of oxazoline RNA-precursors in UV-rich prebiotic environments. *Chemical Communications*, **2018**, 54, 13407-13410	5.8	9
57	Molecules in confinement in liquid solvents: general discussion. *Faraday Discussions*, **2018**, 212, 383-397	3.6	1
56	Electron-driven proton transfer enables nonradiative photodeactivation in microhydrated 2-aminoimidazole. *Faraday Discussions*, **2018**, 212, 345-358	3.6	3
55	Solvation effects alter the photochemistry of 2-thiocytosine. *Chemical Physics*, **2018**, 515, 502-508	2.3	8
54	Water-chromophore electron transfer determines the photochemistry of cytosine and cytidine. *Physical Chemistry Chemical Physics*, **2017**, 19, 17531-17537	3.6	16
53	A prebiotically plausible synthesis of pyrimidine β-ribonucleosides and their phosphate derivatives involving photoanomerization. *Nature Chemistry*, **2017**, 9, 303-309	17.6	81
52	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. *Physical Chemistry Chemical Physics*, **2016**, 18, 22467-77	3.6	10

51	Ultrafast excited-state dynamics of isocytosine. *Physical Chemistry Chemical Physics*, **2016**, 18, 20208-18	3.6	27
50	Photorelaxation of imidazole and adenine via electron-driven proton transfer along HO wires. *Faraday Discussions*, **2016**, 195, 237-251	3.6	11
49	Prebiotic synthesis of nucleic acids and their building blocks at the atomic level - merging models and mechanisms from advanced computations and experiments. *Physical Chemistry Chemical Physics*, **2016**, 18, 20047-66	3.6	40
48	On the particular importance of vibrational contributions to the static electrical properties of model linear molecules under spatial confinement. *Physical Chemistry Chemical Physics*, **2015**, 17, 21782-6	3.6	16
47	Distributed Multipolar Expansion Approach to Calculation of Excitation Energy Transfer Couplings. *Journal of Chemical Theory and Computation*, **2015**, 11, 3259-66	6.4	19
46	Electron-Driven Proton Transfer Along H2O Wires Enables Photorelaxation of States in Chromophore-Water Clusters. *Journal of Physical Chemistry Letters*, **2015**, 6, 1467-71	6.4	29
45	Excited-state hydrogen atom abstraction initiates the photochemistry of 2Rdeoxycytidine. *Chemical Science*, **2015**, 6, 2035-2043	9.4	14
44	Solvent effects on the photochemistry of 4-aminoimidazole-5-carbonitrile, a prebiotically plausible precursor of purines. *Physical Chemistry Chemical Physics*, **2014**, 16, 17617-26	3.6	12
43	Molecular mechanism of diaminomaleonitrile to diaminofumaronitrile photoisomerization: an intermediate step in the prebiotic formation of purine nucleobases. *Chemistry - A European Journal*, **2014**, 20, 2515-21	4.8	8
42	On the origins of large interaction-induced first hyperpolarizabilities in hydrogen-bonded electronic complexes. *Journal of Physical Chemistry A*, **2013**, 117, 6859-66	2.8	11
41	Photochemistry of 2-Aminooxazole, a Hypothetical Prebiotic Precursor of RNA Nucleotides. *Journal of Physical Chemistry Letters*, **2013**, 4, 2785-2788	6.4	28
40	How does the Boys and Bernardi counterpoise correction scheme affects the calculated interaction-induced electric properties? Model hydrogen-bonded systems as a case study. *Chemical Physics Letters*, **2013**, 571, 28-33	2.5	9
39	Induced optical activity of DNA-templated cyanine dye aggregates: exciton coupling theory and TD-DFT studies. *Journal of Physical Chemistry A*, **2013**, 117, 5909-18	2.8	12
38	Resonance-assisted hydrogen bonds revisited. Resonance stabilization vs. charge delocalization. *Physical Chemistry Chemical Physics*, **2013**, 15, 2514-22	3.6	58
37	Theoretical studies of the mechanism of 2-aminooxazole formation under prebiotically plausible conditions. *Physical Chemistry Chemical Physics*, **2013**, 15, 7812-8	3.6	12
36	The effect of intermolecular interactions on the electric dipole polarizabilities of nucleic acid base complexes. *Chemical Physics Letters*, **2013**, 555, 230-234	2.5	14
35	On the performance of long-range-corrected density functional theory and reduced-size polarized LPol-n basis sets in computations of electric dipole (hyper)polarizabilities of conjugated molecules. *Journal of Computational Chemistry*, **2013**, 34, 819-26	3.5	24
34	Resonant and Nonresonant Hyperpolarizabilities of Spatially Confined Molecules: A Case Study of Cyanoacetylene. *Journal of Chemical Theory and Computation*, **2013**, 9, 3463-72	6.4	25

33	The theoretical studies of interactions of the OH(H2O)n clusters evolution toward the hydroxide anion hydration. *International Journal of Quantum Chemistry*, **2012**, 112, 3046-3051	2.1	2
32	On the calculations of interaction energies and induced electric properties within the polarizable continuum model. *Journal of Physical Chemistry A*, **2012**, 116, 4409-16	2.8	20
31	Electric dipole (hyper)polarizabilities of spatially confined LiH molecule. *Journal of Chemical Physics*, **2012**, 137, 094307	3.9	25
30	Electronic structure, bonding, spectra, and linear and nonlinear electric properties of Ti@C28. *Journal of Physical Chemistry A*, **2011**, 115, 10370-81	2.8	33
29	Large changes of static electric properties induced by hydrogen bonding: an ab initio study of linear HCN oligomers. *Journal of Physical Chemistry A*, **2011**, 115, 4691-700	2.8	23
28	The Ethidium-UA/AU Intercalation Site: Effect of Model Fragmentation and Backbone Charge State. *Journal of Chemical Theory and Computation*, **2011**, 7, 2600-9	6.4	8
27	Structural variability and the nature of intermolecular interactions in Watson-Crick B-DNA base pairs. *Journal of Physical Chemistry B*, **2010**, 114, 9629-44	3.4	34
26	On the nature of intermolecular interactions in nucleic acid base-amino acid side-chain complexes. *Journal of Physical Chemistry B*, **2009**, 113, 11511-20	3.4	20
25	On decomposition of interaction-induced electric properties of HF dimer. *Chemical Physics Letters*, **2008**, 461, 203-206	2.5	19
24	On the cooperativity of the interaction-induced (hyper)polarizabilities of the selected hydrogen-bonded trimers. *Chemical Physics Letters*, **2007**, 436, 116-123	2.5	60
23	The nature of interactions in uracil dimer: An ab initio study. *Chemical Physics Letters*, **2007**, 450, 132-137	2.5	25
22	On the influence of microsolvation by argon atoms on the electron affinity properties of water dimer. *Journal of Chemical Physics*, **2006**, 124, 94304	3.9	0
21	On the weak intermolecular interactions and their influence on the optical properties of unsaturated hydrocarbons. Part 1: Two-body interactions. *Molecular Physics*, **2006**, 104, 2263-2271	1.7	5
20	Proton bound open shell systems. Theoretical studies on O2H+(O2)n (n = 1–5) complexes. *Molecular Physics*, **2006**, 104, 2327-2336	1.7	2
19	The nature of interactions in the ionic crystal of 3-pentenenitrile, 2-nitro-5-oxo, ion(-1), sodium. *Journal of Physical Chemistry B*, **2005**, 109, 2027-33	3.4	36
18	Dimers of formic acid, acetic acid, formamide and pyrrole-2-carboxylic acid: an ab initio study. *Journal of Physical Chemistry A*, **2005**, 109, 6397-405	2.8	144
17	On the influence of non-additive interactions on the optical properties of the selected subsystems of crystalline urea. *Chemical Physics Letters*, **2005**, 406, 29-37	2.5	19
16	Intermolecular interactions in solution: elucidating the influence of the solvent. *Journal of Chemical Physics*, **2004**, 120, 2802-13	3.9	39

15	Theoretical ab initio study on the electronic states of GaO and Ga2O. *Computational and Theoretical Chemistry*, **2004**, 672, 105-111		5
14	The micro-solvation of Na+: theoretical study of bonding characteristics in weakly bonded ArnNa+ (n=1–8) clusters. *Chemical Physics Letters*, **2004**, 391, 112-119	2.5	12
13	Molecular properties of protonated homogeneous and mixed carbon oxide and carbon dioxide clusters. *Journal of Chemical Physics*, **2003**, 119, 6560-6570	3.9	8
12	A new theoretical insight into the nature of intermolecular interactions in the molecular crystal of urea. *Journal of Chemical Physics*, **2002**, 117, 1031-1039	3.9	74
11	Bonding in the oxo ferrous iron species: A complete active-space self-consistent-field theory verification of the molecular-oxygen-like pattern. *Journal of Chemical Physics*, **2002**, 117, 7153-7161	3.9	17
10	The Molecular Structures, Energetics, and Nature of Interactions in Arn-N2H+ (n = 1–12) Complexes. *Journal of Physical Chemistry A*, **2002**, 106, 11162-11167	2.8	16
9	The structures and properties of cis- and trans-MeCl2(NH3)2, Me=Pd and Pt complexes, in ground and excited states*. *International Journal of Quantum Chemistry*, **2001**, 83, 213-219	2.1	8
8	The influence of the detachment of electrons on the properties and the nature of interactions in X–H2O (X=Cl, Br) complexes. *Journal of Chemical Physics*, **2001**, 115, 3469-3473	3.9	10
7	The molecular structures and nature of interactions in CH3+Arn(n=1–8) complexes. *Journal of Chemical Physics*, **2001**, 115, 771-777	3.9	17
6	New theoretical insight into the thermal cis–trans isomerization of azo compounds: Protonation lowers the activation barrier. *Journal of Chemical Physics*, **2001**, 114, 5504-5508	3.9	42
5	I–H2O and its neutral precursors: Similarities and differences. *Journal of Chemical Physics*, **2001**, 115, 9260-9265	3.9	18
4	Properties and nature of interactions in Cl(H2O)nn=1,6 clusters: a theoretical study. *Chemical Physics Letters*, **2000**, 325, 7-14	2.5	52
3	C–H···π interactions involving acetylene: an ab initio MO study. *Journal of Molecular Structure*, **2000**, 556, 315-320	3.4	23
2	A theoretical study of the structures and energetics of O2Ar (n=1–8) clusters. *Chemical Physics Letters*, **1999**, 313, 198-204	2.5	16
1	Structure and Nature of the Interaction of the CH3N2+Ion Shellvated by H2Molecules: CH3N2+(H2)n=1-9. *Journal of Physical Chemistry A*, **1999**, 103, 9138-9143	2.8	8