

# Robert W Gra

## List of Publications by Citations

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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	Dimers of formic acid, acetic acid, formamide and pyrrole-2-carboxylic acid: an ab initio study. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 6397-405	2.8	144
67	A prebiotically plausible synthesis of pyrimidine Ribonucleosides and their phosphate derivatives involving photoanomerization. <i>Nature Chemistry</i> , <b>2017</b> , 9, 303-309	17.6	81
66	A new theoretical insight into the nature of intermolecular interactions in the molecular crystal of urea. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 1031-1039	3.9	74
65	On the cooperativity of the interaction-induced (hyper)polarizabilities of the selected hydrogen-bonded trimers. <i>Chemical Physics Letters</i> , <b>2007</b> , 436, 116-123	2.5	60
64	Resonance-assisted hydrogen bonds revisited. Resonance stabilization vs. charge delocalization. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 2514-22	3.6	58
63	Selective prebiotic formation of RNA pyrimidine and DNA purine nucleosides. <i>Nature</i> , <b>2020</b> , 582, 60-66	50.4	52
62	Properties and nature of interactions in Cl(H <sub>2</sub> O) <sub>n</sub> =1,6 clusters: a theoretical study. <i>Chemical Physics Letters</i> , <b>2000</b> , 325, 7-14	2.5	52
61	New theoretical insight into the thermal cis-trans isomerization of azo compounds: Protonation lowers the activation barrier. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 5504-5508	3.9	42
60	Prebiotic synthesis of nucleic acids and their building blocks at the atomic level - merging models and mechanisms from advanced computations and experiments. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 20047-66	3.6	40
59	Intermolecular interactions in solution: elucidating the influence of the solvent. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 2802-13	3.9	39
58	The nature of interactions in the ionic crystal of 3-pentenenitrile, 2-nitro-5-oxo, ion(-1), sodium. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 2027-33	3.4	36
57	Structural variability and the nature of intermolecular interactions in Watson-Crick B-DNA base pairs. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 9629-44	3.4	34
56	Electronic structure, bonding, spectra, and linear and nonlinear electric properties of Ti@C <sub>28</sub> . <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 10370-81	2.8	33
55	Electron-Driven Proton Transfer Along H <sub>2</sub> O Wires Enables Photorelaxation of $\pi$ States in Chromophore-Water Clusters. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 1467-71	6.4	29
54	Photochemistry of 2-Aminooxazole, a Hypothetical Prebiotic Precursor of RNA Nucleotides. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 2785-2788	6.4	28
53	Ultrafast excited-state dynamics of isocytosine. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 20208-18	3.6	27
52	Resonant and Nonresonant Hyperpolarizabilities of Spatially Confined Molecules: A Case Study of Cyanoacetylene. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 3463-72	6.4	25

51	Electric dipole (hyper)polarizabilities of spatially confined LiH molecule. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 094307	3.9	25
50	The nature of interactions in uracil dimer: An ab initio study. <i>Chemical Physics Letters</i> , <b>2007</b> , 450, 132-137.	2.5	25
49	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 $\pi$ -conjugated molecules. <i>Journal of Computational Chemistry</i> , <b>2013</b> , 34, 819-26	3.5	24
48	Large changes of static electric properties induced by hydrogen bonding: an ab initio study of linear HCN oligomers. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 4691-700	2.8	23
47	$\text{C}\equiv\text{N}\cdots\text{N}$ interactions involving acetylene: an ab initio MO study. <i>Journal of Molecular Structure</i> , <b>2000</b> , 556, 315-320	3.4	23
46	On the calculations of interaction energies and induced electric properties within the polarizable continuum model. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 4409-16	2.8	20
45	On the nature of intermolecular interactions in nucleic acid base-amino acid side-chain complexes. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 11511-20	3.4	20
44	Distributed Multipolar Expansion Approach to Calculation of Excitation Energy Transfer Couplings. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 3259-66	6.4	19
43	On decomposition of interaction-induced electric properties of HF dimer. <i>Chemical Physics Letters</i> , <b>2008</b> , 461, 203-206	2.5	19
42	On the influence of non-additive interactions on the optical properties of the selected subsystems of crystalline urea. <i>Chemical Physics Letters</i> , <b>2005</b> , 406, 29-37	2.5	19
41	$\text{H}_2\text{O}$ and its neutral precursors: Similarities and differences. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 9260-9265	3.9	18
40	The molecular structures and nature of interactions in $\text{CH}_3+\text{Ar}_n(n=1-8)$ complexes. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 771-777	3.9	17
39	Bonding in the oxo ferrous iron species: A complete active-space self-consistent-field theory verification of the molecular-oxygen-like pattern. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 7153-7161	3.9	17
38	Water-chromophore electron transfer determines the photochemistry of cytosine and cytidine. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 17531-17537	3.6	16
37	On the particular importance of vibrational contributions to the static electrical properties of model linear molecules under spatial confinement. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 21782-8	3.6	16
36	The Molecular Structures, Energetics, and Nature of Interactions in $\text{Ar}_n\text{-N}_2\text{H}^+$ ( $n = 1-2$ ) Complexes. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 11162-11167	2.8	16
35	A theoretical study of the structures and energetics of $\text{OAr}_n$ ( $n=1-8$ ) clusters. <i>Chemical Physics Letters</i> , <b>1999</b> , 313, 198-204	2.5	16
34	The effect of intermolecular interactions on the electric dipole polarizabilities of nucleic acid base complexes. <i>Chemical Physics Letters</i> , <b>2013</b> , 555, 230-234	2.5	14

33	Excited-state hydrogen atom abstraction initiates the photochemistry of 2-deoxycytidine. <i>Chemical Science</i> , <b>2015</b> , 6, 2035-2043	9.4	14
32	Solvent effects on the photochemistry of 4-aminoimidazole-5-carbonitrile, a prebiotically plausible precursor of purines. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 17617-26	3.6	12
31	Induced optical activity of DNA-templated cyanine dye aggregates: exciton coupling theory and TD-DFT studies. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 5909-18	2.8	12
30	Theoretical studies of the mechanism of 2-aminooxazole formation under prebiotically plausible conditions. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 7812-8	3.6	12
29	The micro-solvation of Na <sup>+</sup> : theoretical study of bonding characteristics in weakly bonded ArnNa <sup>+</sup> (n=18) clusters. <i>Chemical Physics Letters</i> , <b>2004</b> , 391, 112-119	2.5	12
28	Photorelaxation of imidazole and adenine via electron-driven proton transfer along HO wires. <i>Faraday Discussions</i> , <b>2016</b> , 195, 237-251	3.6	11
27	On the origins of large interaction-induced first hyperpolarizabilities in hydrogen-bonded electronic complexes. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 6859-66	2.8	11
26	Applications of Thermal Activation, Ball-milling and Aqueous Medium in Stereoselective Michael Addition of Nitromethane to Enynones Catalyzed by Chiral Squaramides. <i>Advanced Synthesis and Catalysis</i> , <b>2019</b> , 361, 1108-1116	5.6	11
25	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 22467-77	3.6	10
24	The influence of the detachment of electrons on the properties and the nature of interactions in XB <sub>2</sub> O (X=Cl, Br) complexes. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 3469-3473	3.9	10
23	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 19841-19849	3.6	9
22	How does the Boys and Bernardi counterpoise correction scheme affects the calculated interaction-induced electric properties? Model hydrogen-bonded systems as a case study. <i>Chemical Physics Letters</i> , <b>2013</b> , 571, 28-33	2.5	9
21	Photostability of oxazoline RNA-precursors in UV-rich prebiotic environments. <i>Chemical Communications</i> , <b>2018</b> , 54, 13407-13410	5.8	9
20	Molecular mechanism of diaminomaleonitrile to diaminofumaronitrile photoisomerization: an intermediate step in the prebiotic formation of purine nucleobases. <i>Chemistry - A European Journal</i> , <b>2014</b> , 20, 2515-21	4.8	8
19	The Ethidium-UA/AU Intercalation Site: Effect of Model Fragmentation and Backbone Charge State. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 2600-9	6.4	8
18	Molecular properties of protonated homogeneous and mixed carbon oxide and carbon dioxide clusters. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 6560-6570	3.9	8
17	The structures and properties of cis- and trans-MeCl <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> , Me=Pd and Pt complexes, in ground and excited states*. <i>International Journal of Quantum Chemistry</i> , <b>2001</b> , 83, 213-219	2.1	8
16	Structure and Nature of the Interaction of the CH <sub>3</sub> N <sub>2</sub> <sup>+</sup> Ion Shellvated by H <sub>2</sub> Molecules: CH <sub>3</sub> N <sub>2</sub> <sup>+</sup> (H <sub>2</sub> ) <sub>n=1-9</sub> . <i>Journal of Physical Chemistry A</i> , <b>1999</b> , 103, 9138-9143	2.8	8

15	Solvation effects alter the photochemistry of 2-thiocytosine. <i>Chemical Physics</i> , <b>2018</b> , 515, 502-508	2.3	8
14	On the weak intermolecular interactions and their influence on the optical properties of unsaturated hydrocarbons. Part 1: Two-body interactions. <i>Molecular Physics</i> , <b>2006</b> , 104, 2263-2271	1.7	5
13	Theoretical ab initio study on the electronic states of GaO and Ga <sub>2</sub> O. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 672, 105-111		5
12	UV-induced hydrogen transfer in DNA base pairs promoted by dark n $\pi$ states. <i>Chemical Communications</i> , <b>2019</b> , 56, 201-204	5.8	4
11	Electron-driven proton transfer enables nonradiative photodeactivation in microhydrated 2-aminoimidazole. <i>Faraday Discussions</i> , <b>2018</b> , 212, 345-358	3.6	3
10	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. II. Halogen-bonded systems. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 4225-4234	3.6	2
9	The theoretical studies of interactions of the OH(H <sub>2</sub> O) <sub>n</sub> clusters evolution toward the hydroxide anion hydration. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 3046-3051	2.1	2
8	Proton bound open shell systems I: theoretical studies on O <sub>2</sub> H <sup>+</sup> (O <sub>2</sub> ) <sub>n</sub> (n = 1 $\bar{8}$ ) complexes. <i>Molecular Physics</i> , <b>2006</b> , 104, 2327-2336	1.7	2
7	Ribose Alters the Photochemical Properties of the Nucleobase in Thionated Nucleosides. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 6707-6713	6.4	1
6	Stereoselectivity Enhancement During the Generation of Three Contiguous Stereocenters in Tetrahydrothiophenes. <i>ChemCatChem</i> , <b>2021</b> , 13, 574-580	5.2	1
5	Molecules in confinement in liquid solvents: general discussion. <i>Faraday Discussions</i> , <b>2018</b> , 212, 383-397	3.6	1
4	Ab initio effective one-electron potential operators: Applications for charge-transfer energy in effective fragment potentials. <i>Journal of Computational Chemistry</i> , <b>2021</b> , 42, 398-411	3.5	1
3	On the influence of microsolvation by argon atoms on the electron affinity properties of water dimer. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 94304	3.9	0
2	Ultrafast nonradiative deactivation of photoexcited 8-oxo-hypoxanthine: a nonadiabatic molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 1234-1241	3.6	0
1	An effective potential for Frenkel excitons. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 1923-1935	3.6	0