Robert W GÃ³ra

List of Publications by Year
in descending order

69	1,665	304368	315357
papers	citations	22 h-index	38 g-index

73	73	73	1626
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dimers of Formic Acid, Acetic Acid, Formamide and Pyrrole-2-carboxylic Acid:â€‰ an Ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 6397-6405.	1.1	157
2	A prebiotically plausible synthesis of pyrimidine Î²-ribonucleosides and their phosphate derivatives involving photoanomerization. Nature Chemistry, 2017, 9, 303-309.	6.6	109
3	Selective prebiotic formation of RNA pyrimidine and DNA purine nucleosides. Nature, 2020, 582, 60-66.	13.7	106
4	A new theoretical insight into the nature of intermolecular interactions in the molecular crystal of urea. Journal of Chemical Physics, 2002, 117, 1031-1039.	1.2	75
5	Resonance-assisted hydrogen bonds revisited. Resonance stabilization vs. charge delocalization. Physical Chemistry Chemical Physics, 2013, 15, 2514.	1.3	71
6	On the cooperativity of the interaction-induced (hyper)polarizabilities of the selected hydrogen-bonded trimers. Chemical Physics Letters, 2007, 436, 116-123.	1.2	63
7	Properties and nature of interactions in Clâ¯(H2O)nn=1,6 clusters: a theoretical study. Chemical Physics Letters, 2000, 325, 7-14.	1.2	54
8	New theoretical insight into the thermal cisâ€“trans isomerization of azo compounds: Protonation lowers the activation barrier. Journal of Chemical Physics, 2001, 114, 5504-5508.	1.2	49
9	Prebiotic synthesis of nucleic acids and their building blocks at the atomic level â€“ merging models and mechanisms from advanced computations and experiments. Physical Chemistry Chemical Physics, 2016, 18, 20047-20066.	1.3	48
10	Structural Variability and the Nature of Intermolecular Interactions in Watsonâ¯Crick B-DNA Base Pairs. Journal of Physical Chemistry B, 2010, 114, 9629-9644.	1.2	42
11	Intermolecular interactions in solution: Elucidating the influence of the solvent. Journal of Chemical Physics, 2004, 120, 2802-2813.	1.2	39
12	The Nature of Interactions in the Ionic Crystal of 3-Pentenenitrile, 2-Nitro-5-oxo, Ion(â¯1), Sodium. Journal of Physical Chemistry B, 2005, 109, 2027-2033.	1.2	38
13	Ultrafast excited-state dynamics of isocytosine. Physical Chemistry Chemical Physics, 2016, 18, 20208-20218.	1.3	34
14	Electronic Structure, Bonding, Spectra, and Linear and Nonlinear Electric Properties of Ti@C₂₈. Journal of Physical Chemistry A, 2011, 115, 10370-10381.	1.1	33
15	Electron-Driven Proton Transfer Along H₂O Wires Enables Photorelaxation of Ï€Ïƒ* States in Chromophoreâ€“Water Clusters. Journal of Physical Chemistry Letters, 2015, 6, 1467-1471.	2.1	31
16	Photochemistry of 2-Aminooxazole, a Hypothetical Prebiotic Precursor of RNA Nucleotides. Journal of Physical Chemistry Letters, 2013, 4, 2785-2788.	2.1	29
17	On the performance of longâ€rangeâ€corrected density functional theory and reducedâ€size polarized LPolâ€n basis sets in computations of electric dipole (hyper)polarizabilities of Ï€â€conjugated molecules. Journal of Computational Chemistry, 2013, 34, 819-826.	1.5	28
18	Electric dipole (hyper)polarizabilities of spatially confined LiH molecule. Journal of Chemical Physics, 2012, 137, 094307.	1.2	27

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19	Resonant and Nonresonant Hyperpolarizabilities of Spatially Confined Molecules: A Case Study of Cyanoacetylene. Journal of Chemical Theory and Computation, 2013, 9, 3463-3472.	2.3	27
20	The nature of interactions in uracil dimer: An ab initio study. Chemical Physics Letters, 2007, 450, 132-137.	1.2	26
21	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, 4691-4700.	1.1	25
22	Câ€“Hâ‹Ï€ interactions involving acetylene: an ab initio MO study. Journal of Molecular Structure, 2000, 556, 315-320.	1.8	23
23	On the Nature of Intermolecular Interactions in Nucleic Acid Baseâˆ'Amino Acid Side-Chain Complexes. Journal of Physical Chemistry B, 2009, 113, 11511-11520.	1.2	22
24	On the Calculations of Interaction Energies and Induced Electric Properties within the Polarizable Continuum Model. Journal of Physical Chemistry A, 2012, 116, 4409-4416.	1.1	22
25	Distributed Multipolar Expansion Approach to Calculation of Excitation Energy Transfer Couplings. Journal of Chemical Theory and Computation, 2015, 11, 3259-3266.	2.3	21
26	Waterâ€“chromophore electron transfer determines the photochemistry of cytosine and cytidine. Physical Chemistry Chemical Physics, 2017, 19, 17531-17537.	1.3	21
27	On decomposition of interaction-induced electric properties of HF dimer. Chemical Physics Letters, 2008, 461, 203-206.	1.2	20
28	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.	1.2	19
29	Iâˆ'H2O and its neutral precursors: Similarities and differences. Journal of Chemical Physics, 2001, 115, 9260-9265.	1.2	18
30	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.	1.2	18
31	Applications of Thermal Activation, Ballâ€milling and Aqueous Medium in Stereoselective Michael Addition of Nitromethane to Enynones Catalyzed by Chiral Squaramides. Advanced Synthesis and Catalysis, 2019, 361, 1108-1116.	2.1	18
32	The molecular structures and nature of interactions in CH3+Arn(n=1â€“8) complexes. Journal of Chemical Physics, 2001, 115, 771-777.	1.2	17
33	The Molecular Structures, Energetics, and Nature of Interactions in Arn-N2H+(n= 1âˆ'12) Complexes. Journal of Physical Chemistry A, 2002, 106, 11162-11167.	1.1	17
34	Excited-state hydrogen atom abstraction initiates the photochemistry of Î²-2â€²-deoxycytidine. Chemical Science, 2015, 6, 2035-2043.	3.7	17
35	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, 21782-21786.	1.3	17
36	A theoretical study of the structures and energetics of Oâˆ'Ar (n=1â€“6) clusters. Chemical Physics Letters, 1999, 313, 198-204.	1.2	16

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37	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. Physical Chemistry Chemical Physics, 2016, 18, 22467-22477.	1.3	16
38	The effect of intermolecular interactions on the electric dipole polarizabilities of nucleic acid base complexes. Chemical Physics Letters, 2013, 555, 230-234.	1.2	15
39	The micro-solvation of Na+: theoretical study of bonding characteristics in weakly bonded ArnNa+ (n=1â€“8) clusters. Chemical Physics Letters, 2004, 391, 112-119.	1.2	14
40	Induced Optical Activity of DNA-Templated Cyanine Dye Aggregates: Exciton Coupling Theory and TD-DFT Studies. Journal of Physical Chemistry A, 2013, 117, 5909-5918.	1.1	13
41	Theoretical studies of the mechanism of 2-aminooxazole formation under prebiotically plausible conditions. Physical Chemistry Chemical Physics, 2013, 15, 7812.	1.3	13
42	Solvent effects on the photochemistry of 4-aminoimidazole-5-carbonitrile, a prebiotically plausible precursor of purines. Physical Chemistry Chemical Physics, 2014, 16, 17617-17626.	1.3	13
43	Molecular Mechanism of Diaminomaleonitrile to Diaminofumaronitrile Photoisomerization: An Intermediate Step in the Prebiotic Formation of Purine Nucleobases. Chemistry - A European Journal, 2014, 20, 2515-2521.	1.7	13
44	Solvation effects alter the photochemistry of 2-thiocytosine. Chemical Physics, 2018, 515, 502-508.	0.9	13
45	The influence of the detachment of electrons on the properties and the nature of interactions in Xâ^'H2Oâ€‰(X=Cl,â€ŠBr) complexes. Journal of Chemical Physics, 2001, 115, 3469-3473.	1.2	12
46	On the Origins of Large Interaction-Induced First Hyperpolarizabilities in Hydrogen-Bonded Ï€-Electronic Complexes. Journal of Physical Chemistry A, 2013, 117, 6859-6866.	1.1	12
47	Photorelaxation of imidazole and adenine via electron-driven proton transfer along H₂O wires. Faraday Discussions, 2016, 195, 237-251.	1.6	12
48	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. Physical Chemistry Chemical Physics, 2018, 20, 19841-19849.	1.3	12
49	Photostability of oxazoline RNA-precursors in UV-rich prebiotic environments. Chemical Communications, 2018, 54, 13407-13410.	2.2	11
50	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.	1.2	9
51	Structure and Nature of the Interaction of the CH3N2+Ion Shellvated by H2Molecules:Â CH3N2+(H2)n=1-9. Journal of Physical Chemistry A, 1999, 103, 9138-9143.	1.1	8
52	The structures and properties ofcis- andtrans-MeCl2(NH3)2, Me=Pd and Pt complexes, in ground and excited states. International Journal of Quantum Chemistry, 2001, 83, 213-219.	1.0	8
53	Molecular properties of protonated homogeneous and mixed carbon oxide and carbon dioxide clusters. Journal of Chemical Physics, 2003, 119, 6560-6570.	1.2	8
54	The Ethidiumâ€“UA/AU Intercalation Site: Effect of Model Fragmentation and Backbone Charge State. Journal of Chemical Theory and Computation, 2011, 7, 2600-2609.	2.3	8

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55	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. II. Halogen-bonded systems. Physical Chemistry Chemical Physics, 2020, 22, 4225-4234.	1.3	8
56	Theoretical ab initio study on the electronic states of GaO and Ga2O. Computational and Theoretical Chemistry, 2004, 672, 105-111.	1.5	7
57	UV-induced hydrogen transfer in DNA base pairs promoted by dark nï€* states. Chemical Communications, 2020, 56, 201-204.	2.2	6
58	Stereoselectivity Enhancement During the Generation of Three Contiguous Stereocenters in Tetrahydrothiophenes. ChemCatChem, 2021, 13, 574-580.	1.8	6
59	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.	0.8	5
60	Ribose Alters the Photochemical Properties of the Nucleobase in Thionated Nucleosides. Journal of Physical Chemistry Letters, 2021, 12, 6707-6713.	2.1	5
61	Proton bound open shell systems â€“ theoretical studies on O2H+(O2)n(nâ€‰=â€‰1â€“6) complexes. Molecular Physics, 2006, 104, 2327-2336.	0.8	3
62	The theoretical studies of interactions of the OH^{â˜}(H₂O)_n clusters evolution toward the hydroxide anion hydration. International Journal of Quantum Chemistry, 2012, 112, 3046-3051.	1.0	3
63	Electron-driven proton transfer enables nonradiative photodeactivation in microhydrated 2-aminoimidazole. Faraday Discussions, 2018, 212, 345-358.	1.6	3
64	Ultrafast nonradiative deactivation of photoexcited 8-oxo-hypoxanthine: a nonadiabatic molecular dynamics study. Physical Chemistry Chemical Physics, 2021, 23, 1234-1241.	1.3	3
65	Photoinduced waterâ€“chromophore electron transfer causes formation of guanosine photodamage. Physical Chemistry Chemical Physics, 2022, 24, 8217-8224.	1.3	3
66	An effective potential for Frenkel excitons. Physical Chemistry Chemical Physics, 2021, 23, 1923-1935.	1.3	2
67	Ab initio effective <scp>oneâ€electron</scp> potential operators: Applications for <scp>chargeâ€transfer</scp> energy in effective fragment potentials. Journal of Computational Chemistry, 2021, 42, 398-411.	1.5	2
68	On the influence of microsolvation by argon atoms on the electron affinity properties of water dimer. Journal of Chemical Physics, 2006, 124, 094304.	1.2	1
69	Molecules in confinement in liquid solvents: general discussion. Faraday Discussions, 2018, 212, 383-397.	1.6	1