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	Photoinduced waterâ€“chromophore electron transfer causes formation of guanosine photodamage. Physical Chemistry Chemical Physics, 2022, 24, 8217-8224.	1.3	3
2	Stereoselectivity Enhancement During the Generation of Three Contiguous Stereocenters in Tetrahydrothiophenes. ChemCatChem, 2021, 13, 574-580.	1.8	6
3	Ultrafast nonradiative deactivation of photoexcited 8-oxo-hypoxanthine: a nonadiabatic molecular dynamics study. Physical Chemistry Chemical Physics, 2021, 23, 1234-1241.	1.3	3
4	An effective potential for Frenkel excitons. Physical Chemistry Chemical Physics, 2021, 23, 1923-1935.	1.3	2
5	Ribose Alters the Photochemical Properties of the Nucleobase in Thionated Nucleosides. Journal of Physical Chemistry Letters, 2021, 12, 6707-6713.	2.1	5
6	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
7	UV-induced hydrogen transfer in DNA base pairs promoted by dark nÏ€* states. Chemical Communications, 2020, 56, 201-204.	2.2	6
8	Selective prebiotic formation of RNA pyrimidine and DNA purine nucleosides. Nature, 2020, 582, 60-66.	13.7	106
9	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
10	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
11	Photostability of oxazoline RNA-precursors in UV-rich prebiotic environments. Chemical Communications, 2018, 54, 13407-13410.	2.2	11
12	Molecules in confinement in liquid solvents: general discussion. Faraday Discussions, 2018, 212, 383-397.	1.6	1
13	Electron-driven proton transfer enables nonradiative photodeactivation in microhydrated 2-aminoimidazole. Faraday Discussions, 2018, 212, 345-358.	1.6	3
14	Solvation effects alter the photochemistry of 2-thiocytosine. Chemical Physics, 2018, 515, 502-508.	0.9	13
15	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
16	Waterâ€“chromophore electron transfer determines the photochemistry of cytosine and cytidine. Physical Chemistry Chemical Physics, 2017, 19, 17531-17537.	1.3	21
17	A prebiotically plausible synthesis of pyrimidine Î²-ribonucleosides and their phosphate derivatives involving photoanomerization. Nature Chemistry, 2017, 9, 303-309.	6.6	109
18	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

#	Article	IF	Citations
19	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. Physical Chemistry Chemical Physics, 2016, 18, 22467-22477.	1.3	16
20	Ultrafast excited-state dynamics of isocytosine. Physical Chemistry Chemical Physics, 2016, 18, 20208-20218.	1.3	34
21	Photorelaxation of imidazole and adenine via electron-driven proton transfer along H₂O wires. Faraday Discussions, 2016, 195, 237-251.	1.6	12
22	Excited-state hydrogen atom abstraction initiates the photochemistry of Î²-2â€²-deoxycytidine. Chemical Science, 2015, 6, 2035-2043.	3.7	17
23	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
24	Distributed Multipolar Expansion Approach to Calculation of Excitation Energy Transfer Couplings. Journal of Chemical Theory and Computation, 2015, 11, 3259-3266.	2.3	21
25	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
26	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
27	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
28	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
29	Photochemistry of 2-Aminooxazole, a Hypothetical Prebiotic Precursor of RNA Nucleotides. Journal of Physical Chemistry Letters, 2013, 4, 2785-2788.	2.1	29
30	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
31	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
32	Resonance-assisted hydrogen bonds revisited. Resonance stabilization vs. charge delocalization. Physical Chemistry Chemical Physics, 2013, 15, 2514.	1.3	71
33	Theoretical studies of the mechanism of 2-aminooxazole formation under prebiotically plausible conditions. Physical Chemistry Chemical Physics, 2013, 15, 7812.	1.3	13
34	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
35	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
36	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

#	Article	IF	Citations
37	Electric dipole (hyper)polarizabilities of spatially confined LiH molecule. Journal of Chemical Physics, 2012, 137, 094307.	1.2	27
38	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
39	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
40	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
41	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
42	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
43	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
44	On the Nature of Intermolecular Interactions in Nucleic Acid Baseâ˜’Amino Acid Side-Chain Complexes. Journal of Physical Chemistry B, 2009, 113, 11511-11520.	1.2	22
45	On decomposition of interaction-induced electric properties of HF dimer. Chemical Physics Letters, 2008, 461, 203-206.	1.2	20
46	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
47	The nature of interactions in uracil dimer: An ab initio study. Chemical Physics Letters, 2007, 450, 132-137.	1.2	26
48	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
49	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
50	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
51	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
52	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
53	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
54	Intermolecular interactions in solution: Elucidating the influence of the solvent. Journal of Chemical Physics, 2004, 120, 2802-2813.	1.2	39

#	Article	IF	Citations
55	Theoretical ab initio study on the electronic states of GaO and Ga2O. Computational and Theoretical Chemistry, 2004, 672, 105-111.	1.5	7
56	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
57	Molecular properties of protonated homogeneous and mixed carbon oxide and carbon dioxide clusters. Journal of Chemical Physics, 2003, 119, 6560-6570.	1.2	8
58	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
59	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
60	The Molecular Structures, Energetics, and Nature of Interactions in Arn-N2H+(n= 1â^’12) Complexes. Journal of Physical Chemistry A, 2002, 106, 11162-11167.	1.1	17
61	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
62	Iâ^’H2O and its neutral precursors: Similarities and differences. Journal of Chemical Physics, 2001, 115, 9260-9265.	1.2	18
63	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
64	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
65	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
66	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
67	Câ€“Hâ‹Ï€ interactions involving acetylene: an ab initio MO study. Journal of Molecular Structure, 2000, 556, 315-320.	1.8	23
68	A theoretical study of the structures and energetics of Oâ^’Ar (n=1â€“6) clusters. Chemical Physics Letters, 1999, 313, 198-204.	1.2	16
69	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