Anil Kumar

List of Publications by Year
in descending order

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53 papers	1,907 citations	257450 24 h-index	254184 43 g-index
55 all docs	55 docs citations	55 times ranked	1281 citing authors

#	Article	IF	Citations
1	Modulation of the Directionality of Hole Transfer between the Base and the Sugar-Phosphate Backbone in DNA with the Number of Sulfur Atoms in the Phosphate Group. Journal of Physical Chemistry B, 2022, 126, 430-442.	2.6	2
2	Proton-Transfer Reactions in One-Electron-Oxidized G-Quadruplexes: A Density Functional Theory Study. Journal of Physical Chemistry B, 2022, 126, 1483-1491.	2.6	3
3	Electron-Induced Repair of 2â€²-Deoxyribose Sugar Radicals in DNA: A Density Functional Theory (DFT) Study. International Journal of Molecular Sciences, 2021, 22, 1736.	4.1	5
4	Temperature Effects on CO₂ Electroreduction Pathways in an Imidazolium-Based Ionic Liquid on Pt Electrode. Journal of Physical Chemistry C, 2020, 124, 26094-26105.	3.1	15
5	Site of Azido Substitution in the Sugar Moiety of Azidopyrimidine Nucleosides Influences the Reactivity of Aminyl Radicals Formed by Dissociative Electron Attachment. Journal of Physical Chemistry B, 2020, 124, 11357-11370.	2.6	4
6	One Way Traffic: Baseâ€toâ€Backbone Hole Transfer in Nucleoside Phosphorodithioate. Chemistry - A European Journal, 2020, 26, 9407-9407.	3.3	0
7	One Way Traffic: Baseâ€toâ€Backbone Hole Transfer in Nucleoside Phosphorodithioate. Chemistry - A European Journal, 2020, 26, 9495-9505.	3.3	4
8	One-electron oxidation of ds(5â€²-GGG-3â€²) and ds(5â€²-G(8OG)G-3â€²) and the nature of hole distribution: a density functional theory (DFT) study. Physical Chemistry Chemical Physics, 2020, 22, 5078-5089.	2.8	15
9	Reaction of Electrons with DNA: Radiation Damage to Radiosensitization. International Journal of Molecular Sciences, 2019, 20, 3998.	4.1	54
10	Adsorption and Electrochemistry of Carbon Monoxide at the Ionic Liquidâ€“Pt Interface. Journal of Physical Chemistry B, 2019, 123, 4726-4734.	2.6	10
11	Excited States of One-Electron Oxidized Guanine-Cytosine Base Pair Radicals: A Time Dependent Density Functional Theory Study. Journal of Physical Chemistry A, 2019, 123, 3098-3108.	2.5	18
12	Observation of dissociative quasi-free electron attachment to nucleoside via excited anion radical in solution. Nature Communications, 2019, 10, 102.	12.8	55
13	Direct observation of the oxidation of DNA bases by phosphate radicals formed under radiation: a model of the backbone-to-base hole transfer. Physical Chemistry Chemical Physics, 2018, 20, 14927-14937.	2.8	20
14	SOMOâ€“HOMO Level Inversion in Biologically Important Radicals. Journal of Physical Chemistry B, 2018, 122, 98-105.	2.6	52
15	Electron-Mediated Aminyl and Iminyl Radicals from C5 Azido-Modified Pyrimidine Nucleosides Augment Radiation Damage to Cancer Cells. Organic Letters, 2018, 20, 7400-7404.	4.6	14
16	Low-Energy Electron (LEE)-Induced DNA Damage: Theoretical Approaches to Modeling Experiment. , 2017, , 1741-1802.		13
17	Hydrogen Electrooxidation in Ionic Liquids Catalyzed by the NTf2 Radical. Journal of Physical Chemistry C, 2017, 121, 5161-5167.	3.1	13
18	Prehydrated One-Electron Attachment to Azido-Modified Pentofuranoses: Aminyl Radical Formation, Rapid H-Atom Transfer, and Subsequent Ring Opening. Journal of Physical Chemistry B, 2017, 121, 4968-4980.	2.6	11

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19	Cytosine Iminyl Radical (cytN^{â€¢}) Formation via Electron-Induced Debromination of 5-Bromocytosine: A DFT and Gaussian 4 Study. Journal of Physical Chemistry A, 2017, 121, 4825-4829.	2.5	9
20	Gamma and ion-beam irradiation of DNA: Free radical mechanisms, electron effects, and radiation chemical track structure. Radiation Physics and Chemistry, 2016, 128, 60-74.	2.8	47
21	Anaerobic Oxidation of Methane to Methyl Radical in NTf₂-Based Ionic Liquids. Journal of Physical Chemistry C, 2016, 120, 13466-13473.	3.1	7
22	Do Solvated Electrons (e_{aq}^{â€“}) Reduce DNA Bases? A Gaussian 4 and Density Functional Theory-Molecular Dynamics Study. Journal of Physical Chemistry B, 2016, 120, 2115-2123.	2.6	43
23	Comment on â€œProton Transfer of Guanine Radical Cations Studied by Time-Resolved Resonance Raman Spectroscopy Combined with Pulse Radiolysisâ€• Journal of Physical Chemistry B, 2016, 120, 2984-2986.	2.6	14
24	Ï€-Radical to Ïƒ-Radical Tautomerization in One-Electron-Oxidized 1-Methylcytosine and Its Analogs. Journal of Physical Chemistry B, 2015, 119, 11496-11505.	2.6	20
25	A Simple ab Initio Model for the Hydrated Electron That Matches Experiment. Journal of Physical Chemistry A, 2015, 119, 9148-9159.	2.5	88
26	Low-Energy Electron (LEE)-Induced DNA Damage: Theoretical Approaches to Modeling Experiment. , 2015, , 1-63.		1
27	Presolvated Electron Reactions with Methyl Acetoacetate: Electron Localization, Proton-Deuteron Exchange, and H-Atom Abstraction. Molecules, 2014, 19, 13486-13497.	3.8	10
28	An ESR and DFT study of hydration of the 2â€²-deoxyuridine-5-yl radical: a possible hydroxyl radical intermediate. Chemical Communications, 2014, 50, 14605-14608.	4.1	15
29	Reactions of 5-methylcytosine cation radicals in DNA and model systems: Thermal deprotonation from the 5-methyl group vs. excited state deprotonation from sugar. International Journal of Radiation Biology, 2014, 90, 433-445.	1.8	10
30	One-Electron Oxidation of Gemcitabine and Analogs: Mechanism of Formation of C3â€² and C2â€² Sugar Radicals. Journal of the American Chemical Society, 2014, 136, 15646-15653.	13.7	15
31	Proton Transfer Induced SOMO-to-HOMO Level Switching in One-Electron Oxidized A-T and G-C Base Pairs: A Density Functional Theory Study. Journal of Physical Chemistry B, 2014, 118, 5453-5458.	2.6	40
32	Ï€- vs Ïƒ-Radical States of One-Electron-Oxidized DNA/RNA Bases: A Density Functional Theory Study. Journal of Physical Chemistry B, 2013, 117, 11623-11632.	2.6	21
33	Formation of Sâ€“Cl Phosphorothioate Adduct Radicals in dsDNA S-Oligomers: Hole Transfer to Guanine vs Disulfide Anion Radical Formation. Journal of the American Chemical Society, 2013, 135, 12827-12838.	13.7	27
34	Excited state proton-coupled electron transfer in 8-oxoG-C and 8-oxoG-A base pairs: a time dependent density functional theory (TD-DFT) study. Photochemical and Photobiological Sciences, 2013, 12, 1328-1340.	2.9	14
35	Hydroxyl Ion Addition to One-Electron Oxidized Thymine: Unimolecular Interconversion of C5 to C6 OH-Adducts. Journal of the American Chemical Society, 2013, 135, 3121-3135.	13.7	42
36	One-Electron Oxidation of Neutral Sugar Radicals of 2â€²-Deoxyguanosine and 2â€²-Deoxythymidine: A Density Functional Theory (DFT) Study. Journal of Physical Chemistry B, 2012, 116, 9409-9416.	2.6	20

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37	Hydroxyl Radical (OH^{â€¢}) Reaction with Guanine in an Aqueous Environment: A DFT Study. Journal of Physical Chemistry B, 2011, 115, 15129-15137.	2.6	92
38	Density Functional Theory Studies of the Extent of Hole Delocalization in One-Electron Oxidized Adenine and Guanine Base Stacks. Journal of Physical Chemistry B, 2011, 115, 4990-5000.	2.6	55
39	Proton-Coupled Electron Transfer in DNA on Formation of Radiation-Produced Ion Radicals. Chemical Reviews, 2010, 110, 7002-7023.	47.7	185
40	Prototropic equilibria in DNA containing one-electron oxidized GC: intra-duplex vs. duplex to solvent deprotonation. Physical Chemistry Chemical Physics, 2010, 12, 5353.	2.8	54
41	Role of Excited States in Lowâ€Energy Electron (LEE) Induced Strand Breaks in DNA Model Systems: Influence of Aqueous Environment. ChemPhysChem, 2009, 10, 1426-1430.	2.1	45
42	Sugar Radical Formation by a Proton Coupled Hole Transfer in 2â€²-Deoxyguanosine Radical Cation (2â€²-dGâ€¢+): A Theoretical Treatment. Journal of Physical Chemistry B, 2009, 113, 13374-13380.	2.6	20
43	Influence of Hydration on Proton Transfer in the Guanineâˆ'Cytosine Radical Cation (G^{â€¢+}âˆ'C) Base Pair: A Density Functional Theory Study. Journal of Physical Chemistry B, 2009, 113, 11359-11361.	2.6	97
44	Effect of Base Stacking on the Acidâˆ'Base Properties of the Adenine Cation Radical [Aâ€¢+] in Solution: ESR and DFT Studies. Journal of the American Chemical Society, 2008, 130, 10282-10292.	13.7	74
45	Photoexcitation of Adenine Cation Radical [Aâ€¢+] in the near UVâˆ'vis Region Produces Sugar Radicals in Adenosine and in Its Nucleotides. Journal of Physical Chemistry B, 2008, 112, 15844-15855.	2.6	36
46	The Role of Ï€Ïƒ* Excited States in Electron-Induced DNA Strand Break Formation:â€‰ A Time-Dependent Density Functional Theory Study. Journal of the American Chemical Society, 2008, 130, 2130-2131.	13.7	71
47	Microhydration of the Guanineâˆ'Cytosine (GC) Base Pair in the Neutral and Anionic Radical States:â€‰ A Density Functional Study. Journal of Physical Chemistry B, 2008, 112, 5189-5198.	2.6	48
48	Formation of Sugar Radicals in RNA Model Systems and Oligomers via Excitation of Guanine Cation Radical. Journal of Physical Chemistry B, 2008, 112, 2168-2178.	2.6	33
49	Radiation Effects On DNA: Theoretical Investigations Of Electron, Hole And Excitation Pathways To DNA Damage. Challenges and Advances in Computational Chemistry and Physics, 2008, , 577-617.	0.6	17
50	Low-Energy Electron Attachment to 5â€˜-Thymidine Monophosphate:Â Modeling Single Strand Breaks Through Dissociative Electron Attachment. Journal of Physical Chemistry B, 2007, 111, 5464-5474.	2.6	81
51	Photo-induced Hole Transfer from Base to Sugar in DNA: Relationship to Primary Radiation Damage. Radiation Research, 2006, 165, 479-484.	1.5	55
52	Photoexcitation of Dinucleoside Radical Cations:Â A Time-Dependent Density Functional Study. Journal of Physical Chemistry B, 2006, 110, 24181-24188.	2.6	45
53	The Guanine Cation Radical:Â Investigation of Deprotonation States by ESR and DFT. Journal of Physical Chemistry B, 2006, 110, 24171-24180.	2.6	133