

Shinichiro Nakamura

List of Publications by Year in descending order

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89
papers

3,462
citations

117453

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143772

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docs citations

90
times ranked

2854
citing authors

#	ARTICLE	IF	CITATIONS
1	A Theoretical Study on Non-Bridging Dimer Formation of a Cationic Platinum Complex with a Redox-Active Ligand. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
2	Photoinduced cytotoxicity of photochromic symmetric diarylethene derivatives: the relation of structure and cytotoxicity. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 3211-3217.	1.5	4
3	Molecular Design Learned from the Natural Product Porphyrin-334: Molecular Generation via Chemical Variational Autoencoder versus Database Mining via Similarity Search, A Comparative Study. <i>ACS Omega</i> , 2022, 7, 8581-8590.	1.6	3
4	Autopolymerization of 2-bromo-3-methoxythiophene, analysis of reaction products and estimation of polymer structure. <i>Polymer Journal</i> , 2021, 53, 429-438.	1.3	1
5	Molecular crystalline capsules that release their contents by light. <i>Chemical Science</i> , 2021, 12, 11585-11592.	3.7	11
6	Carrier Pathway for Photoelectrochemical Water Oxidation with Intermediate State in n-type GaN Compared with Route of Anodic Corrosion. <i>Journal of Physical Chemistry C</i> , 2021, 125, 8562-8569.	1.5	1
7	Spontaneous Combustion of 2-Bromo-3-Methoxythiophene: A Study on Reaction Pathways and Energetics by Quantum Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5615-5625.	1.1	0
8	Determining Factor of the Quantum Yield of the Cyclization Reaction via Triplet States for Dye-Attached Diarylethene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5895-5902.	1.1	7
9	Photoinduced topographical surface changes and photoresponse of the crystals of 7-methoxycoumarin. <i>CrystEngComm</i> , 2021, 23, 5780-5787.	1.3	3
10	Excitation light intensity dependence of 2.2 eV yellow photoluminescence of n-type GaN. <i>Japanese Journal of Applied Physics</i> , 2021, 60, 011002.	0.8	2
11	Photoinduced swing of a diarylethene thin broad sword shaped crystal: a study on the detailed mechanism. <i>Chemical Science</i> , 2020, 11, 12307-12315.	3.7	29
12	Cyclization from Higher Excited States of Diarylethenes Having a Substituted Azulene Ring. <i>Chemistry - A European Journal</i> , 2020, 26, 11441-11450.	1.7	3
13	Biomimetic Functions by Microscopic Molecular Reactions in Macroscopic Photoresponsive Crystalline System. , 2020, , 405-425.		0
14	A comparison of geometries and electronic structure of plumbogummite (PbAl ₃ P ₂ O ₁₄ H ₆), Pb ₂ P ₄ O ₁₂ and Pb ₂ P ₂ O ₇ . <i>Chemical Physics Letters</i> , 2020, 756, 137800.	1.2	0
15	Dual wettability on diarylethene microcrystalline surface mimicking a termite wing. <i>Communications Chemistry</i> , 2019, 2, .	2.0	13
16	Unique Structural Relaxations and Molecular Conformations of Porphyrin-334 at the Excited State. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7649-7656.	1.2	13
17	Object Transportation System Mimicking the Cilia of Paramecium aurelia Making Use of the Light-Controllable Crystal Bending Behavior of a Photochromic Diarylethene. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13308-13312.	7.2	27
18	Investigation of a Pathway for Water Delivery in Photosystem II Protein by Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6444-6452.	1.2	10

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19	Aggregation-induced emission effect on turn-off fluorescent switching of a photochromic diarylethene. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 2204-2212.	1.3	7
20	Structural analysis of a novel lipooligosaccharide (LOS) from <i>Rhodobacter azotoformans</i> . <i>Carbohydrate Research</i> , 2019, 473, 104-114.	1.1	6
21	First principles calculations of surface dependent electronic structures: a study on $\hat{1}^2$ -FeOOH and $\hat{1}^3$ -FeOOH. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18486-18494.	1.3	17
22	Photosalient Effect of Diarylethene Crystals of Thiazoyl and Thienyl Derivatives. <i>Chemistry - A European Journal</i> , 2019, 25, 7874-7880.	1.7	40
23	Effect of Atomic Charges on Octanol's Water Partition Coefficient Using Alchemical Free Energy Calculation. <i>Molecules</i> , 2018, 23, 425.	1.7	16
24	Investigation of carrier transfer mechanism of NiO-loaded n-type GaN photoanodic reaction for water oxidation by comparison between band model and optical measurements. <i>MRS Communications</i> , 2018, 8, 480-486.	0.8	6
25	Effects of NiO-loading on n-type GaN photoanode for photoelectrochemical water splitting using different aqueous electrolytes. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 9493-9499.	3.8	22
26	How seaweeds release the excess energy from sunlight to surrounding sea water. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15745-15753.	1.3	17
27	Chemical Insights from Theoretical Electronic States in Nickel Hydroxide and Monolayer Surface Model. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24603-24611.	1.5	5
28	A study on an unusual SN2 mechanism in the methylation of benzyne through nickel-complexation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26926-26933.	1.3	4
29	Photosalient Phenomena that Mimic <i>Impatiens</i> Are Observed in Hollow Crystals of Diarylethene with a Perfluorocyclohexene Ring. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 12576-12580.	7.2	79
30	Unusual Ionic Bond and Solubility Mechanism of NaPQQ ($n = 0-4$) Crystals. <i>Crystal Growth and Design</i> , 2017, 17, 4118-4123.	1.4	5
31	Structural changes in the S3 state of the oxygen evolving complex in photosystem II. <i>Chemical Physics Letters</i> , 2016, 651, 243-250.	1.2	17
32	Legitimate intermediates of oxygen evolution on iridium oxide revealed by in situ electrochemical evanescent wave spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15199-15204.	1.3	40
33	Fractal Surfaces of Molecular Crystals Mimicking Lotus Leaf with Phototunable Double Roughness Structures. <i>Journal of the American Chemical Society</i> , 2016, 138, 10299-10303.	6.6	63
34	Photosalient Effect of a Diarylethene with a Perfluorocyclohexene Ring. <i>Chemistry - A European Journal</i> , 2016, 22, 12680-12683.	1.7	51
35	Photoinduced topographical changes on microcrystalline surfaces of diarylethenes. <i>CrystEngComm</i> , 2016, 18, 7229-7235.	1.3	10
36	Momentum-dependent band spin splitting in semiconducting MnO_2 : a density functional calculation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13294-13303.	1.3	39

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37	Mechanism of glycine oxidation catalyzed by pyrroloquinoline quinone in aqueous solution. <i>Chemical Physics Letters</i> , 2015, 620, 13-18.	1.2	3
38	Quality Assessment of Predicted Protein Models Using Energies Calculated by the Fragment Molecular Orbital Method. <i>Molecular Informatics</i> , 2015, 34, 97-104.	1.4	13
39	Activation of CO ₂ by ionic liquid EMIM ⁺ BF ₄ ⁻ in the electrochemical system: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23521-23531.	1.3	101
40	A diarylethene as the SO ₂ gas generator upon UV irradiation. <i>Chemical Communications</i> , 2015, 51, 1736-1738.	2.2	24
41	Theoretical Study on the Role of Ca ²⁺ at the S ₂ State in Photosystem II. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14215-14222.	1.2	30
42	Derivatives of the approximated electrostatic potentials in unrestricted Hartree-Fock based on the fragment molecular orbital method and an application to polymer radicals. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	16
43	Octahedral point-charge model and its application to fragment molecular orbital calculations of chemical shifts. <i>Chemical Physics Letters</i> , 2014, 593, 165-173.	1.2	18
44	Potential Energy Surfaces and Quantum Yields for Photochromic Diarylethene Reactions. <i>Molecules</i> , 2013, 18, 5091-5103.	1.7	28
45	Tuning the Temperature Dependence for Switching in Dithienylethene Photochromic Switches. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8222-8229.	1.1	43
46	All-Atom Molecular Dynamics Simulation of Photosystem II Embedded in Thylakoid Membrane. <i>Journal of the American Chemical Society</i> , 2013, 135, 15670-15673.	6.6	82
47	Analytic second derivatives of the energy in the fragment molecular orbital method. <i>Journal of Chemical Physics</i> , 2013, 138, 164103.	1.2	40
48	Photoinduced Self-Epitaxial Crystal Growth of a Diarylethene Derivative with Antireflection Moth-Eye and Superhydrophobic Lotus Effects. <i>Langmuir</i> , 2013, 29, 8164-8169.	1.6	26
49	Characteristics of hydrogen generation from water splitting by polymer electrolyte electrochemical cell directly connected with concentrated photovoltaic cell. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 14424-14432.	3.8	89
50	Over 12% Light to Hydrogen Energy Conversion Efficiency of Hydrogen Generation from Water: New System Concept, Concentrated Photovoltaic Electrochemical Cell (CPEC). <i>Materials Research Society Symposia Proceedings</i> , 2013, 1491, 52.	0.1	1
51	Theoretical Study on the Photocyclization Mechanism of Diarylethenes with Transition-Metal Substituents. <i>Bulletin of the Chemical Society of Japan</i> , 2012, 85, 679-686.	2.0	4
52	Photochromism of a Diarylethene Having an Azulene Ring. <i>Journal of Organic Chemistry</i> , 2012, 77, 3270-3276.	1.7	39
53	Photochromism of 1,2-Bis(2-thienyl)perfluorocyclopentene Derivatives: Substituent Effect on the Reactive Carbon Atoms. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10973-10979.	1.1	22
54	Photoinduced Formation of Superhydrophobic Surface on Which Contact Angle of a Water Droplet Exceeds 170° by Reversible Topographical Changes on a Diarylethene Microcrystalline Surface. <i>Langmuir</i> , 2012, 28, 17817-17824.	1.6	31

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55	Reversible Photocontrol of Surface Wettability between Hydrophilic and Superhydrophobic Surfaces on an Asymmetric Diarylethene Solid Surface. <i>Langmuir</i> , 2011, 27, 6395-6400.	1.6	64
56	Photo- and electro-chromic organometallics with dithienylethene (DTE) linker, L2CpM-DTE-MCpL2: Dually stimuli-responsive molecular switch. <i>Dalton Transactions</i> , 2011, 40, 10643.	1.6	49
57	Photochromism of diarylethene: Effect of polymer environment and effects on surfaces. <i>Journal of Photochemistry and Photobiology C: Photochemistry Reviews</i> , 2011, 12, 138-150.	5.6	19
58	Phototunable Diarylethene Microcrystalline Surfaces: Lotus and Petal Effects upon Wetting. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 5942-5944.	7.2	105
59	Photo-induced reversible topographical changes of photochromic dithienylethene microcrystalline surfaces. <i>New Journal of Chemistry</i> , 2009, 33, 1324.	1.4	19
60	Metal atom behavior on photochromic diarylethene surfaces—deposition rate dependence of selective Mg deposition. <i>New Journal of Chemistry</i> , 2009, 33, 1335.	1.4	18
61	Unusual Photochromic Behavior of C3-Methoxy-Substituted Bis(2-thienyl)perfluorocyclopentene. <i>Bulletin of the Chemical Society of Japan</i> , 2009, 82, 1441-1446.	2.0	10
62	Theoretical investigation on photochromic diarylethene: A short review. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2008, 200, 10-18.	2.0	72
63	Photoresponsive rolling and bending of thin crystals of chiral diarylethenes. <i>Chemical Communications</i> , 2008, , 326-328.	2.2	138
64	Selective Metal Deposition on Photoswitchable Molecular Surfaces. <i>Journal of the American Chemical Society</i> , 2008, 130, 10740-10747.	6.6	74
65	Formation mechanism of fractal structures on wax surfaces with reference to their super water-repellency. <i>Soft Matter</i> , 2008, 4, 140-144.	1.2	32
66	Super Water-Repellent Fractal Surfaces of a Photochromic Diarylethene Induced by UV Light. <i>Japanese Journal of Applied Physics</i> , 2008, 47, 7298.	0.8	18
67	Photochromism of Diarylethene Single Molecules in Polymer Matrices. <i>Journal of the American Chemical Society</i> , 2007, 129, 5932-5938.	6.6	157
68	Quantum yields and potential energy surfaces: a theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 821-829.	0.9	57
69	Substituent effect of diarylethenes on IR spectra for application of non-destructive readout of photochromic recording. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 998-1006.	0.9	18
70	Hole-injection isomerization of photochromic diarylethene for organic molecular memory. <i>Applied Physics Letters</i> , 2006, 89, 222102.	1.5	36
71	Characterization of Cationic Diarylethene by Electron Spin Resonance and Absorption Spectra Ratio of Open/Closed-Ring Isomers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8137-8143.	1.1	35
72	Direct Observation of Cation Radicals of a Diarylethene during Oxidative Ring-opening Reaction. <i>Chemistry Letters</i> , 2006, 35, 900-901.	0.7	14

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73	Photoinduced Reversible Formation of Microfibrils on a Photochromic Diarylethene Microcrystalline Surface. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 6470-6473.	7.2	126
74	Micrometer-Scale Photochromic Recording on Amorphous Diarylethene Film and Nondestructive Readout Using Near-Field IR Light. <i>Japanese Journal of Applied Physics</i> , 2006, 45, 7114-7120.	0.8	12
75	Three Bits Eight States Photochromic Recording and Nondestructive Readout by Using IR Light. <i>Chemistry - A European Journal</i> , 2005, 11, 534-542.	1.7	76
76	Theoretical Study on the Photochromic Cycloreversion Reactions of Dithienylethenes; on the Role of the Conical Intersections. <i>Journal of the American Chemical Society</i> , 2004, 126, 12112-12120.	6.6	114
77	First-principles study of salicylideneaniline molecular crystals: Tautomerization reaction involving intermolecular hydrogen bonds. <i>Physical Review B</i> , 2004, 69, .	1.1	16
78	Theoretical study on novel quantum yields of dithienylethenes cyclization reactions in crystals. <i>Computational and Theoretical Chemistry</i> , 2003, 625, 227-234.	1.5	23
79	Rotational Isomerization of Dithienylethenes: A Study on the Mechanism Determining Quantum Yield of Cyclization Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4982-4988.	1.1	44
80	Efficient Photocycloreversion Reaction of Diarylethenes by Introduction of Cyano Substituents to the Reactive Carbons. <i>Chemistry Letters</i> , 2003, 32, 858-859.	0.7	38
81	Absorption Spectra of Colored Isomer of Diarylethene in Single Crystals. <i>Chemistry Letters</i> , 2002, 31, 1224-1225.	0.7	37
82	An ab Initio MO Study of the Photochromic Reaction of Dithienylethenes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7222-7227.	1.1	117
83	Theoretical study of an intermediate, a factor determining the quantum yield in photochromism of diarylethene derivatives. <i>Computational and Theoretical Chemistry</i> , 2002, 579, 115-120.	1.5	55
84	Raman spectroscopic study on photochromic reaction of a diarylethene derivative. <i>Chemical Physics Letters</i> , 2002, 357, 113-118.	1.2	27
85	Multiphoton Gated Photochromic Reaction in a Diarylethene Derivative. <i>Journal of the American Chemical Society</i> , 2001, 123, 753-754.	6.6	95
86	Substitution Effect on the Coloration Quantum Yield of a Photochromic Bisbenzothienylethene. <i>Chemistry Letters</i> , 1999, 28, 63-64.	0.7	156
87	Photochromism of dinaphthylethene derivatives. Stability of the closed-ring forms. <i>Research on Chemical Intermediates</i> , 1995, 21, 861-876.	1.3	57
88	Thermally Irreversible Photochromic Systems. Substituent Effect on the Absorption Wavelength of 11,12-Dicyano-5a,5b-dihydro-5a,5b-dimethylbenzo[1,2-b:6,5-b'â€²]bis[1]benzothiophene. <i>Bulletin of the Chemical Society of Japan</i> , 1992, 65, 430-435.	2.0	44
89	Thermally irreversible photochromic systems. A theoretical study. <i>Journal of Organic Chemistry</i> , 1988, 53, 6136-6138.	1.7	308