

Dongwook Kim

List of Publications by Year in descending order

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101384

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95
all docs

95
docs citations

95
times ranked

6240
citing authors

#	ARTICLE	IF	CITATIONS
1	Up-Conversion Intersystem Crossing Rates in Organic Emitters for Thermally Activated Delayed Fluorescence: Impact of the Nature of Singlet vs Triplet Excited States. <i>Journal of the American Chemical Society</i> , 2017, 139, 4042-4051.	6.6	698
2	Understanding of Assembly Phenomena by Aromatic π -Aromatic Interactions: A Benzene Dimer and the Substituted Systems. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3446-3457.	1.1	617
3	Thermally Activated Delayed Fluorescence (TADF) Path toward Efficient Electroluminescence in Purely Organic Materials: Molecular Level Insight. <i>Accounts of Chemical Research</i> , 2018, 51, 2215-2224.	7.6	382
4	Theoretical Investigations of Anion π - π Interactions: The Role of Anions and the Nature of π Systems. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1250-1258.	1.1	260
5	Cation π - π Interactions: A Theoretical Investigation of the Interaction of Metallic and Organic Cations with Alkenes, Arenes, and Heteroarenes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1228-1238.	1.1	226
6	Substituent Effects on the Edge-to-Face Aromatic Interactions. <i>Journal of the American Chemical Society</i> , 2005, 127, 4530-4537.	6.6	190
7	Complete basis set limit of <i>ab initio</i> binding energies and geometrical parameters for various typical types of complexes. <i>Journal of Computational Chemistry</i> , 2008, 29, 1208-1221.	1.5	144
8	Structures, spectra, and electronic properties of halide-water pentamers and hexamers, $X_n(H_2O)_{5,6}$ ($X=F, Cl, Br, I$): <i>Ab initio</i> study. <i>Journal of Chemical Physics</i> , 2002, 116, 5509-5520.	1.2	135
9	Use of X-Ray Diffraction, Molecular Simulations, and Spectroscopy to Determine the Molecular Packing in a Polymer-Fullerene Bimolecular Crystal. <i>Advanced Materials</i> , 2012, 24, 6071-6079.	11.1	126
10	Excimers Beyond Pyrene: A Far-Red Optical Proximity Reporter and its Application to the Label-Free Detection of DNA. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 3912-3916.	7.2	126
11	Triplet Excimer Formation in Platinum-Based Phosphors: A Theoretical Study of the Roles of Pt π -Pt Bimetallic Interactions and Interligand π - π Interactions. <i>Journal of the American Chemical Society</i> , 2009, 131, 11371-11380.	6.6	121
12	Design of Efficient Ambipolar Host Materials for Organic Blue Electrophosphorescence: Theoretical Characterization of Hosts Based on Carbazole Derivatives. <i>Journal of the American Chemical Society</i> , 2011, 133, 17895-17900.	6.6	116
13	Effect of π -conjugated bridges of TPD-based medium bandgap conjugated copolymers for efficient tandem organic photovoltaic cells. <i>Energy and Environmental Science</i> , 2014, 7, 4118-4131.	15.6	115
14	Three-Dimensional Packing Structure and Electronic Properties of Biaxially Oriented Poly(2,5-bis(3-alkylthiophene-2-yl)thieno[3,2- <i>b</i>]thiophene) Films. <i>Journal of the American Chemical Society</i> , 2012, 134, 6177-6190.	6.6	108
15	Assembling Phenomena of Calix[4]hydroquinone Nanotube Bundles by One-Dimensional Short Hydrogen Bonding and Displaced π - π Stacking. <i>Journal of the American Chemical Society</i> , 2002, 124, 14268-14279.	6.6	106
16	Cation π -Anion Interaction: A Theoretical Investigation of the Role of Induction Energies. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7980-7986.	1.1	101
17	Phosphine Oxide Derivatives as Hosts for Blue Phosphors: A Joint Theoretical and Experimental Study of Their Electronic Structure. <i>Chemistry of Materials</i> , 2010, 22, 247-254.	3.2	95
18	Thiophene-rich fused-aromatic thienopyrazine acceptor for donor-acceptor low band-gap polymers for OTFT and polymer solar cell applications. <i>Journal of Materials Chemistry</i> , 2010, 20, 5823.	6.7	84

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19	Mechanistic insight into the sensing of nitroaromatic compounds by metal-organic frameworks. <i>Communications Chemistry</i> , 2019, 2, .	2.0	82
20	Theoretical Investigation of Normal to Strong Hydrogen Bonds. <i>Structural Chemistry</i> , 2005, 16, 187-202.	1.0	66
21	Norbornene-Based Copolymers Containing Platinum Complexes and Bis(carbazolyl)benzene Groups in Their Side-Chains. <i>Macromolecules</i> , 2009, 42, 6855-6864.	2.2	66
22	Local-Excitation versus Charge-Transfer Characters in the Triplet State: Theoretical Insight into the Singlet-Triplet Energy Differences of Carbazolyl-Phthalonitrile-Based Thermally Activated Delayed Fluorescence Materials. <i>Journal of Physical Chemistry C</i> , 2016, 120, 28330-28336.	1.5	58
23	Simple Bithiophene-Rhodanine-Based Small Molecule Acceptor for Use in Additive-Free Nonfullerene OPVs with Low Energy Loss of 0.51 eV. <i>Advanced Energy Materials</i> , 2019, 9, 1804021.	10.2	58
24	An Electrochemically Controllable Nanomechanical Molecular System Utilizing Edge-to-Face and Face-to-Face Aromatic Interactions. <i>Organic Letters</i> , 2002, 4, 3971-3974.	2.4	56
25	Electronic Structure of Carbazole-Based Phosphine Oxides as Ambipolar Host Materials for Deep Blue Electrophosphorescence: A Density Functional Theory Study. <i>Chemistry of Materials</i> , 2012, 24, 2604-2610.	3.2	56
26	High open circuit voltage organic photovoltaic cells fabricated using 9,9-bifluorenylidene as a non-fullerene type electron acceptor. <i>Chemical Communications</i> , 2013, 49, 10950.	2.2	55
27	Theoretical Investigation of Triscarbazole Derivatives As Host Materials for Blue Electrophosphorescence: Effects of Topology. <i>Chemistry of Materials</i> , 2011, 23, 5223-5230.	3.2	53
28	Spin-Vibronic Model for Quantitative Prediction of Reverse Intersystem Crossing Rate in Thermally Activated Delayed Fluorescence Systems. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 621-632.	2.3	53
29	Catalytic Mechanism of Enzymes: Preorganization, Short Strong Hydrogen Bond, and Charge Buffering. <i>Biochemistry</i> , 2002, 41, 5300-5306.	1.2	52
30	Topology analysis of metal-organic frameworks based on metal-organic polyhedra as secondary or tertiary building units. <i>Inorganic Chemistry Frontiers</i> , 2015, 2, 336-360.	3.0	52
31	Three States Involving Vibronic Resonance is a Key to Enhancing Reverse Intersystem Crossing Dynamics of an Organoboron-Based Ultrapure Blue Emitter. <i>Jacs Au</i> , 2021, 1, 987-997.	3.6	48
32	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metal-Organic Polyhedra. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1041-1045.	7.2	45
33	Effects of Intermolecular Interactions on the Singlet-Triplet Energy Difference: A Theoretical Study of the Formation of Excimers in Acene Molecules. <i>Journal of Physical Chemistry C</i> , 2015, 119, 12690-12697.	1.5	42
34	Non-halogenated solvent-processed ternary-blend solar cells via alkyl-side-chain engineering of a non-fullerene acceptor and their application in large-area devices. <i>Journal of Materials Chemistry A</i> , 2020, 8, 10318-10330.	5.2	39
35	Rational Design of Biologically Important Chemosensors: A Novel Receptor for Selective Recognition of Acetylcholine over Ammonium Cations. <i>Organic Letters</i> , 2003, 5, 471-474.	2.4	38
36	Exploring Gas-Phase Ion-Ionophore Interactions: Infrared Spectroscopy of Argon-Tagged Alkali Ion-Crown Ether Complexes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1514-1520.	1.1	37

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37	Theoretical Investigation of Hyperthermal Reactions at the Gas-Liquid Interface: O ₂ (3P) and Squalane. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5019-5031.	1.1	36
38	Controlling the Morphology of BDTT-DPP-Based Small Molecules via End-Group Functionalization for Highly Efficient Single and Tandem Organic Photovoltaic Cells. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 23866-23875.	4.0	33
39	Yellow-Colored Electro-Optic Crystals as Intense Terahertz Wave Sources. <i>Advanced Functional Materials</i> , 2018, 28, 1801143.	7.8	32
40	Homochiral Asymmetric C-Shaped Electron-Transporting Materials for Efficient Non-Fullerene Perovskite Solar Cells. <i>ChemSusChem</i> , 2019, 12, 224-230.	3.6	32
41	DPP-based small molecule, non-fullerene acceptors for channel charge generation in OPVs and their improved performance in ternary cells. <i>RSC Advances</i> , 2015, 5, 4811-4821.	1.7	31
42	Chemical Stabilities of the Lowest Triplet State in Aryl Sulfones and Aryl Phosphine Oxides Relevant to OLED Applications. <i>Chemistry of Materials</i> , 2019, 31, 1507-1519.	3.2	29
43	Metal-organic framework based on hinged cube tessellation as transformable mechanical metamaterial. <i>Science Advances</i> , 2019, 5, eaav4119.	4.7	28
44	Efficient Optical-to-THz Conversion Organic Crystals with Simultaneous Electron Withdrawing and Donating Halogen Substituents. <i>Advanced Optical Materials</i> , 2018, 6, 1700930.	3.6	27
45	New Electro-Optic Salt Crystals for Efficient Terahertz Wave Generation by Direct Pumping at Ti:Sapphire Wavelength. <i>Advanced Optical Materials</i> , 2017, 5, 1600758.	3.6	26
46	A Single-Benzene-Based Fluorophore: Optical Waveguiding in the Crystal Form. <i>ChemPlusChem</i> , 2019, 84, 1130-1134.	1.3	26
47	A New Type of Ionophore Family Utilizing the Cation-Olefinic π -Interaction: A Theoretical Study of [n]Beltenes. <i>Journal of Organic Chemistry</i> , 2002, 67, 1848-1851.	1.7	24
48	Hydrated hydride anion clusters. <i>Journal of Chemical Physics</i> , 2007, 127, 164311.	1.2	22
49	Symmetry-guided syntheses of mixed-linker Zr metal-organic frameworks with precise linker locations. <i>Chemical Science</i> , 2019, 10, 5801-5806.	3.7	22
50	A theoretical understanding of the energy difference between singlet and triplet states of oligoacene molecules. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 651-655.	1.0	21
51	Drastic change of magnetic anisotropy in Fe ₃ GeTe ₂ and Fe ₄ GeTe ₂ monolayers under electric field studied by density functional theory. <i>Scientific Reports</i> , 2021, 11, 17567.	1.6	20
52	Topology Conversions of Non-Interpenetrated Metal-Organic Frameworks to Doubly Interpenetrated Metal-Organic Frameworks. <i>Chemistry of Materials</i> , 2017, 29, 3899-3907.	3.2	17
53	Organic π -Hole Containing Crystals with Enhanced Nonlinear Optical Response and Efficient Optical-to-THz Frequency Conversion. <i>Advanced Optical Materials</i> , 2020, 8, 1901840.	3.6	17
54	A Theoretical Analysis of the Excited State of Oligoacene Aggregates: Local Excitation vs. Charge-Transfer Transition. <i>Bulletin of the Korean Chemical Society</i> , 2015, 36, 2284-2289.	1.0	16

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55	Wide-Bandgap Organic Crystals: Enhanced Optical-to-Terahertz Nonlinear Frequency Conversion at Near-Infrared Pumping. <i>Advanced Optical Materials</i> , 2020, 8, 1902099.	3.6	15
56	Efficient Gap-Free Broadband Terahertz Generators Based on New Organic Quinolinium Single Crystals. <i>Advanced Optical Materials</i> , 2019, 7, 1900953.	3.6	14
57	Gas-Induced Ion-Free Stable Radical Anion Formation of Organic Semiconducting Solids as Highly Gas-Selective Probes. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 35904-35913.	4.0	14
58	Transformation of a Cluster-Based Metal-Organic Framework to a Rod Metal-Organic Framework. <i>Chemistry of Materials</i> , 2022, 34, 273-278.	3.2	14
59	Theoretical studies on hydroquinone-benzene clusters. <i>Journal of Chemical Physics</i> , 2005, 122, 014305.	1.2	13
60	Modeling Reactive Scattering of F_2 at a Liquid Squalane Interface: A Hybrid QM/MM Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7218-7226.	1.1	13
61	Molecular salt crystals with bis(head-to-tail) interionic complementary assembly for efficient organic THz generators. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10078-10085.	2.7	13
62	A Theoretical Study of the Formation of Benzene Excimer: Effects of Geometry Relaxation and Spin-state Dependence. <i>Bulletin of the Korean Chemical Society</i> , 2014, 35, 2738-2742.	1.0	13
63	Forming a three-dimensional porous organic network via solid-state explosion of organic single crystals. <i>Nature Communications</i> , 2017, 8, 1599.	5.8	12
64	Fluorinated Organic Electro-Optic Quinolinium Crystals for THz Wave Generation. <i>Advanced Optical Materials</i> , 2019, 7, 1801495.	3.6	12
65	High-Density Organic Electro-Optic Crystals for Ultra-Broadband THz Spectroscopy. <i>Advanced Optical Materials</i> , 2021, 9, 2100618.	3.6	12
66	Temperature dependent CO ₂ behavior in microporous 1-D channels of a metal-organic framework with multiple interaction sites. <i>Scientific Reports</i> , 2017, 7, 41447.	1.6	11
67	A Theoretical Study of Benzene Dimers in the Excited States: Wavefunction Delocalization, Charge-Transfer Admixture, and Electronic Coupling. <i>Bulletin of the Korean Chemical Society</i> , 2017, 38, 763-771.	1.0	11
68	Phonon-Suppressing Intermolecular Adhesives: Catechol-Based Broadband Organic THz Generators. <i>Advanced Science</i> , 2022, 9, .	5.6	11
69	Pseudopolymorphs of LB30870, a Direct Thrombin Inhibitor: One-Dimensional Solvent Channel Structures Explain Reversible Hydration/Dehydration. <i>Crystal Growth and Design</i> , 2018, 18, 95-104.	1.4	10
70	Organic THz Generators: A Design Strategy for Organic Crystals with Ultralarge Macroscopic Hyperpolarizability. <i>Advanced Optical Materials</i> , 2021, 9, 2100324.	3.6	10
71	Direct observation of kink evolution due to Hund's coupling on approach to metal-insulator transition in NiS ₂ xSex. <i>Nature Communications</i> , 2021, 12, 1208.	5.8	9
72	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metal-Organic Polyhedra. <i>Angewandte Chemie</i> , 2019, 131, 1053-1057.	1.6	8

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73	Halides with Fifteen Aliphatic C-H...Anion Interaction Sites. <i>Scientific Reports</i> , 2016, 6, 30123.	1.6	7
74	Effect of Perturbative Vibronic Correction for Weak Fluorescence in Thermally Activated Delayed Fluorescence Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10384-10392.	1.1	7
75	Unusually Stable Triazine-based Organic Superstructures. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 7413-7417.	7.2	6
76	Reversible Single-Crystal-to-Single-Crystal Transformations of Metal-Organic Frameworks that Accompany Two-Dimensional Framework Reorganizations. <i>Crystal Growth and Design</i> , 2017, 17, 2228-2237.	1.4	6
77	Theoretical Study of the Gas Phase Sc + (NO, O2) → ScO + (N, O) Reactions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9600-9605.	1.1	5
78	Theoretical Approaches to the Design of Functional Nanomaterials. <i>Theoretical and Computational Chemistry</i> , 2004, 15, 119-170.	0.2	5
79	New N-pyrimidinyl stilbazolium crystals for second-order nonlinear optics. <i>Optics and Laser Technology</i> , 2022, 156, 108454.	2.2	5
80	A Density Functional Theory Study of Side Chains Effects on the Intermolecular Interactions and Electronic Structures of Small Molecular Acceptors for Organic Photovoltaics. <i>Bulletin of the Korean Chemical Society</i> , 2016, 37, 1244-1252.	1.0	4
81	Role of the Geometry Restriction and Quasi-Degeneracy of the Excited States in Thermally Activated Delayed Fluorescence: A Density Functional Theory Study of Carbazolyl-Bispyridinylmethanone Derivatives. <i>ChemPhotoChem</i> , 2019, 3, 874-880.	1.5	4
82	Design Strategy of Highly Efficient Nonlinear Optical Orange-Colored Crystals with Two Electron-Withdrawing Groups. <i>Advanced Photonics Research</i> , 2022, 3, .	1.7	4
83	Unusually Stable Triazine-based Organic Superstructures. <i>Angewandte Chemie</i> , 2016, 128, 7539-7543.	1.6	3
84	A Density Functional Theory Study of an Exciplex: Pyridine and Benzene. <i>Bulletin of the Korean Chemical Society</i> , 2018, 39, 882-886.	1.0	3
85	Effect of Topology on the Singlet-Triplet Energy Difference and their Natures: A Density Functional Theory Study of Carbazolyl-Phthalonitrile Derivatives. <i>Bulletin of the Korean Chemical Society</i> , 2017, 38, 899-903.	1.0	2
86	A Density Functional Theory Study of an Exciplex II: Benzene and Tricyanobenzene. <i>Bulletin of the Korean Chemical Society</i> , 2019, 40, 735-739.	1.0	2
87	A theoretical study of carbazole dimers: Does carbazole form an excimer that undermines the performance of organic light emitting diodes?. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26363.	1.0	1
88	Pore space partition of a fragile Ag(I)-carboxylate framework via post-synthetic linker insertion. <i>Chemical Communications</i> , 2020, 56, 8615-8618.	2.2	1
89	Nonlinear Optics: New Electro-Optic Salt Crystals for Efficient Terahertz Wave Generation by Direct Pumping at Ti:Sapphire Wavelength (<i>Advanced Optical Materials</i> 5/2017). <i>Advanced Optical Materials</i> , 2017, 5, .	3.6	0