Dongwook Kim

List of Publications by Year in descending order

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89	5,448	101384	82410
papers	citations	36 h-index	72 g-index

95	95	95	6240
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Design Strategy of Highly Efficient Nonlinear Optical Orangeâ€Colored Crystals with Two Electronâ€Withdrawing Groups. Advanced Photonics Research, 2022, 3, .	1.7	4
2	Transformation of a Cluster-Based Metalâ€“Organic Framework to a Rod Metalâ€“Organic Framework. Chemistry of Materials, 2022, 34, 273-278.	3.2	14
3	Phononâ€Suppressing Intermolecular Adhesives: Catecholâ€Based Broadband Organic THz Generators. Advanced Science, 2022, 9, .	5.6	11
4	New N-pyrimidinyl stilbazolium crystals for second-order nonlinear optics. Optics and Laser Technology, 2022, 156, 108454.	2.2	5
5	Direct observation of kink evolution due to Hundâ€™s coupling on approach to metal-insulator transition in NiS2â^'xSex. Nature Communications, 2021, 12, 1208.	5.8	9
6	Organic THz Generators: A Design Strategy for Organic Crystals with Ultralarge Macroscopic Hyperpolarizability. Advanced Optical Materials, 2021, 9, 2100324.	3.6	10
7	Three States Involving Vibronic Resonance is a Key to Enhancing Reverse Intersystem Crossing Dynamics of an Organoboron-Based Ultrapure Blue Emitter. Jacs Au, 2021, 1, 987-997.	3.6	48
8	Highâ€Density Organic Electroâ€Optic Crystals for Ultraâ€Broadband THz Spectroscopy. Advanced Optical Materials, 2021, 9, 2100618.	3.6	12
9	Drastic change of magnetic anisotropy in Fe3GeTe2 and Fe4GeTe2 monolayers under electric field studied by density functional theory. Scientific Reports, 2021, 11, 17567.	1.6	20
10	Spinâ€“Vibronic Model for Quantitative Prediction of Reverse Intersystem Crossing Rate in Thermally Activated Delayed Fluorescence Systems. Journal of Chemical Theory and Computation, 2020, 16, 621-632.	2.3	53
11	A theoretical study of carbazole dimers: Does carbazole form an excimer that undermines the performance of organic light emitting diodes?. International Journal of Quantum Chemistry, 2020, 120, e26363.	1.0	1
12	Effect of Perturbative Vibronic Correction for Weak Fluorescence in Thermally Activated Delayed Fluorescence Systems. Journal of Physical Chemistry A, 2020, 124, 10384-10392.	1.1	7
13	Pore space partition of a fragile Ag(i)-carboxylate framework via post-synthetic linker insertion. Chemical Communications, 2020, 56, 8615-8618.	2.2	1
14	Wideâ€Bandgap Organic Crystals: Enhanced Opticalâ€toâ€Terahertz Nonlinear Frequency Conversion at Nearâ€Infrared Pumping. Advanced Optical Materials, 2020, 8, 1902099.	3.6	15
15	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. Journal of Materials Chemistry A, 2020, 8, 10318-10330.	5.2	39
16	Molecular salt crystals with bis(head-to-tail) interionic complementary assembly for efficient organic THz generators. Journal of Materials Chemistry C, 2020, 8, 10078-10085.	2.7	13
17	Organic Ïƒâ€Hole Containing Crystals with Enhanced Nonlinear Optical Response and Efficient Opticalâ€toâ€THz Frequency Conversion. Advanced Optical Materials, 2020, 8, 1901840.	3.6	17
18	Efficient Gapâ€Free Broadband Terahertz Generators Based on New Organic Quinolinium Single Crystals. Advanced Optical Materials, 2019, 7, 1900953.	3.6	14

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19	A Singleâ€Benzeneâ€Based Fluorophore: Optical Waveguiding in the Crystal Form. ChemPlusChem, 2019, 84, 1130-1134.	1.3	26
20	A Density Functional Theory Study of an Exciplex II: Benzene and Tricyanobenzene. Bulletin of the Korean Chemical Society, 2019, 40, 735-739.	1.0	2
21	Fluorinated Organic Electroâ€Optic Quinolinium Crystals for THz Wave Generation. Advanced Optical Materials, 2019, 7, 1801495.	3.6	12
22	Gas-Induced Ion-Free Stable Radical Anion Formation of Organic Semiconducting Solids as Highly Gas-Selective Probes. ACS Applied Materials & Interfaces, 2019, 11, 35904-35913.	4.0	14
23	Symmetry-guided syntheses of mixed-linker Zr metalâ€“organic frameworks with precise linker locations. Chemical Science, 2019, 10, 5801-5806.	3.7	22
24	Metal-organic framework based on hinged cube tessellation as transformable mechanical metamaterial. Science Advances, 2019, 5, eaav4119.	4.7	28
25	Role of the Geometry Restriction and Quasiâ€Degeneracy of the Excited States in Thermally Activated Delayed Fluorescence: A Density Functional Theory Study of Carbzolylâ€Bispyridinylmethanone Derivatives. ChemPhotoChem, 2019, 3, 874-880.	1.5	4
26	Simple Bithiopheneâ€“Rhodanineâ€Based Small Molecule Acceptor for Use in Additiveâ€Free Nonfullerene OPVs with Low Energy Loss of 0.51 eV. Advanced Energy Materials, 2019, 9, 1804021.	10.2	58
27	Mechanistic insight into the sensing of nitroaromatic compounds by metal-organic frameworks. Communications Chemistry, 2019, 2, .	2.0	82
28	Chemical Stabilities of the Lowest Triplet State in Aryl Sulfones and Aryl Phosphine Oxides Relevant to OLED Applications. Chemistry of Materials, 2019, 31, 1507-1519.	3.2	29
29	Homochiral Asymmetricâ€Shaped Electronâ€Transporting Materials for Efficient Nonâ€Fullerene Perovskite Solar Cells. ChemSusChem, 2019, 12, 224-230.	3.6	32
30	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metalâ€“Organic Polyhedra. Angewandte Chemie, 2019, 131, 1053-1057.	1.6	8
31	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metalâ€“Organic Polyhedra. Angewandte Chemie - International Edition, 2019, 58, 1041-1045.	7.2	45
32	Pseudopolymorphs of LB30870, a Direct Thrombin Inhibitor: One-Dimensional Solvent Channel Structures Explain Reversible Hydration/Dehydration. Crystal Growth and Design, 2018, 18, 95-104.	1.4	10
33	Efficient Opticalâ€toâ€THz Conversion Organic Crystals with Simultaneous Electron Withdrawing and Donating Halogen Substituents. Advanced Optical Materials, 2018, 6, 1700930.	3.6	27
34	Yellowâ€Colored Electroâ€Optic Crystals as Intense Terahertz Wave Sources. Advanced Functional Materials, 2018, 28, 1801143.	7.8	32
35	Thermally Activated Delayed Fluorescence (TADF) Path toward Efficient Electroluminescence in Purely Organic Materials: Molecular Level Insight. Accounts of Chemical Research, 2018, 51, 2215-2224.	7.6	382
36	A Density Functional Theory Study of an Exciplex: Pyridine and Benzene. Bulletin of the Korean Chemical Society, 2018, 39, 882-886.	1.0	3

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37	Temperature dependent CO2 behavior in microporous 1-D channels of a metal-organic framework with multiple interaction sites. Scientific Reports, 2017, 7, 41447.	1.6	11
38	New Electroâ€Optic Salt Crystals for Efficient Terahertz Wave Generation by Direct Pumping at Ti:Sapphire Wavelength. Advanced Optical Materials, 2017, 5, 1600758.	3.6	26
39	Up-Conversion Intersystem Crossing Rates in Organic Emitters for Thermally Activated Delayed Fluorescence: Impact of the Nature of Singlet vs Triplet Excited States. Journal of the American Chemical Society, 2017, 139, 4042-4051.	6.6	698
40	Nonlinear Optics: New Electroâ€Optic Salt Crystals for Efficient Terahertz Wave Generation by Direct Pumping at Ti:Sapphire Wavelength (Advanced Optical Materials 5/2017). Advanced Optical Materials, 2017, 5, .	3.6	0
41	Topology Conversions of Non-Interpenetrated Metalâ€“Organic Frameworks to Doubly Interpenetrated Metalâ€“Organic Frameworks. Chemistry of Materials, 2017, 29, 3899-3907.	3.2	17
42	A Theoretical Study of Benzene Dimers in the Excited States: Wavefunction Delocalization, Chargeâ€Transfer Admixture, and Electronic Coupling. Bulletin of the Korean Chemical Society, 2017, 38, 763-771.	1.0	11
43	Reversible Single-Crystal-to-Single-Crystal Transformations of Metalâ€“Organic Frameworks that Accompany Two-Dimensional Framework Reorganizations. Crystal Growth and Design, 2017, 17, 2228-2237.	1.4	6
44	Effect of Topology on the Singletâ€“Triplet Energy Difference and their Natures: A Density Functional Theory Study of Carbazolylâ€Phthalonitrile Derivatives. Bulletin of the Korean Chemical Society, 2017, 38, 899-903.	1.0	2
45	Forming a three-dimensional porous organic network via solid-state explosion of organic single crystals. Nature Communications, 2017, 8, 1599.	5.8	12
46	A theoretical understanding of the energy difference between singlet and triplet states of oligoacene molecules. International Journal of Quantum Chemistry, 2016, 116, 651-655.	1.0	21
47	Unusually Stable Triazineâ€based Organic Superstructures. Angewandte Chemie, 2016, 128, 7539-7543.	1.6	3
48	Halides with Fifteen Aliphatic Câ€“HÂ·Â·Â·Anion Interaction Sites. Scientific Reports, 2016, 6, 30123.	1.6	7
49	Local-Excitation versus Charge-Transfer Characters in the Triplet State: Theoretical Insight into the Singletâ€“Triplet Energy Differences of Carbazolyl-Phthalonitrile-Based Thermally Activated Delayed Fluorescence Materials. Journal of Physical Chemistry C, 2016, 120, 28330-28336.	1.5	58
50	A Density Functional Theory Study of Side Chains Effects on the Intermolecular Interactions and Electronic Structures of Small Molecular Acceptors for Organic Photovoltaics. Bulletin of the Korean Chemical Society, 2016, 37, 1244-1252.	1.0	4
51	Unusually Stable Triazineâ€based Organic Superstructures. Angewandte Chemie - International Edition, 2016, 55, 7413-7417.	7.2	6
52	A Theoretical Analysis of the Excited State of Oligoacene Aggregates: Local Excitation vs. Chargeâ€Transfer Transition. Bulletin of the Korean Chemical Society, 2015, 36, 2284-2289.	1.0	16
53	Excimers Beyond Pyrene: A Farâ€Red Optical Proximity Reporter and its Application to the Labelâ€Free Detection of DNA. Angewandte Chemie - International Edition, 2015, 54, 3912-3916.	7.2	126
54	Topology analysis of metalâ€“organic frameworks based on metalâ€“organic polyhedra as secondary or tertiary building units. Inorganic Chemistry Frontiers, 2015, 2, 336-360.	3.0	52

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55	Effects of Intermolecular Interactions on the Singletâ€“Triplet Energy Difference: A Theoretical Study of the Formation of Excimers in Acene Molecules. Journal of Physical Chemistry C, 2015, 119, 12690-12697.	1.5	42
56	Controlling the Morphology of BDTT-DPP-Based Small Molecules via End-Group Functionalization for Highly Efficient Single and Tandem Organic Photovoltaic Cells. ACS Applied Materials & Interfaces, 2015, 7, 23866-23875.	4.0	33
57	DPP-based small molecule, non-fullerene acceptors for â€œchannel IIâ€•charge generation in OPVs and their improved performance in ternary cells. RSC Advances, 2015, 5, 4811-4821.	1.7	31
58	Effect of Ï€-conjugated bridges of TPD-based medium bandgap conjugated copolymers for efficient tandem organic photovoltaic cells. Energy and Environmental Science, 2014, 7, 4118-4131.	15.6	115
59	A Theoretical Study of the Formation of Benzene Excimer: Effects of Geometry Relaxation and Spin-state Dependence. Bulletin of the Korean Chemical Society, 2014, 35, 2738-2742.	1.0	13
60	High open circuit voltage organic photovoltaic cells fabricated using 9,9â€²-bifluorenylidene as a non-fullerene type electron acceptor. Chemical Communications, 2013, 49, 10950.	2.2	55
61	Electronic Structure of Carbazole-Based Phosphine Oxides as Ambipolar Host Materials for Deep Blue Electrophosphorescence: A Density Functional Theory Study. Chemistry of Materials, 2012, 24, 2604-2610.	3.2	56
62	Use of Xâ€Ray Diffraction, Molecular Simulations, and Spectroscopy to Determine the Molecular Packing in a Polymerâ€Fullerene Bimolecular Crystal. Advanced Materials, 2012, 24, 6071-6079.	11.1	126
63	Three-Dimensional Packing Structure and Electronic Properties of Biaxially Oriented Poly(2,5-bis(3-alkylthiophene-2-yl)thieno[3,2-b]thiophene) Films. Journal of the American Chemical Society, 2012, 134, 6177-6190.	6.6	108
64	Theoretical Investigation of Triscarbazole Derivatives As Host Materials for Blue Electrophosphorescence: Effects of Topology. Chemistry of Materials, 2011, 23, 5223-5230.	3.2	53
65	Design of Efficient Ambipolar Host Materials for Organic Blue Electrophosphorescence: Theoretical Characterization of Hosts Based on Carbazole Derivatives. Journal of the American Chemical Society, 2011, 133, 17895-17900.	6.6	116
66	Exploring Gas-Phase Ionâˆ’Ionophore Interactions: Infrared Spectroscopy of Argon-Tagged Alkali Ion-Crown Ether Complexes. Journal of Physical Chemistry A, 2010, 114, 1514-1520.	1.1	37
67	Thiophene-rich fused-aromatic thienopyrazine acceptor for donorâ€“acceptor low band-gap polymers for OTFT and polymer solar cell applications. Journal of Materials Chemistry, 2010, 20, 5823.	6.7	84
68	Phosphine Oxide Derivatives as Hosts for Blue Phosphors: A Joint Theoretical and Experimental Study of Their Electronic Structure. Chemistry of Materials, 2010, 22, 247-254.	3.2	95
69	Modeling Reactive Scattering of F(²P) at a Liquid Squalane Interface: A Hybrid QM/MM Molecular Dynamics Study. Journal of Physical Chemistry A, 2009, 113, 7218-7226.	1.1	13
70	Triplet Excimer Formation in Platinum-Based Phosphors: A Theoretical Study of the Roles of Ptâˆ’Pt Bimetallic Interactions and Interligand Ï€âˆ’Ï€ Interactions. Journal of the American Chemical Society, 2009, 131, 11371-11380.	6.6	121
71	Norbornene-Based Copolymers Containing Platinum Complexes and Bis(carbazolyl)benzene Groups in Their Side-Chains. Macromolecules, 2009, 42, 6855-6864.	2.2	66
72	Complete basis set limit of Ab initio binding energies and geometrical parameters for various typical types of complexes. Journal of Computational Chemistry, 2008, 29, 1208-1221.	1.5	144

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73	Hydrated hydride anion clusters. Journal of Chemical Physics, 2007, 127, 164311.	1.2	22
74	Theoretical Investigation of Hyperthermal Reactions at the Gasâ^'Liquid Interface:â€‰ O (3P) and Squalane. Journal of Physical Chemistry A, 2007, 111, 5019-5031.	1.1	36
75	Cationâ^'Ï€â^'Anion Interaction:â€‰ A Theoretical Investigation of the Role of Induction Energies. Journal of Physical Chemistry A, 2007, 111, 7980-7986.	1.1	101
76	Understanding of Assembly Phenomena by Aromaticâ^'Aromatic Interactions:Â Benzene Dimer and the Substituted Systems. Journal of Physical Chemistry A, 2007, 111, 3446-3457.	1.1	617
77	Theoretical Investigation of Normal to Strong Hydrogen Bonds. Structural Chemistry, 2005, 16, 187-202.	1.0	66
78	Substituent Effects on the Edge-to-Face Aromatic Interactions. Journal of the American Chemical Society, 2005, 127, 4530-4537.	6.6	190
79	Theoretical studies on hydroquinone-benzene clusters. Journal of Chemical Physics, 2005, 122, 014305.	1.2	13
80	Theoretical Approaches to the Design of Functional Nanomaterials. Theoretical and Computational Chemistry, 2004, 15, 119-170.	0.2	5
81	Theoretical Investigations of Anionâ^'Ï€ Interactions:â€‰ The Role of Anions and the Nature of Ï€ Systems. Journal of Physical Chemistry A, 2004, 108, 1250-1258.	1.1	260
82	Cationâ^'Ï€ Interactions:â€‰ A Theoretical Investigation of the Interaction of Metallic and Organic Cations with Alkenes, Arenes, and Heteroarenes. Journal of Physical Chemistry A, 2003, 107, 1228-1238.	1.1	226
83	Rational Design of Biologically Important Chemosensors:â€‰ A Novel Receptor for Selective Recognition of Acetylcholine over Ammonium Cations. Organic Letters, 2003, 5, 471-474.	2.4	38
84	Theoretical Study of the Gas Phase Sc + (NO, O2) â†' ScO + (N, O) Reactions. Journal of Physical Chemistry A, 2002, 106, 9600-9605.	1.1	5
85	Catalytic Mechanism of Enzymes:Â Preorganization, Short Strong Hydrogen Bond, and Charge Bufferingâ€. Biochemistry, 2002, 41, 5300-5306.	1.2	52
86	Assembling Phenomena of Calix[4]hydroquinone Nanotube Bundles by One-Dimensional Short Hydrogen Bonding and Displaced Ï€â^'Ï€ Stacking. Journal of the American Chemical Society, 2002, 124, 14268-14279.	6.6	106
87	A New Type of Ionophore Family Utilizing the Cation-Olefinic Ï€ Interaction:Â Theoretical Study of [n]Beltenes. Journal of Organic Chemistry, 2002, 67, 1848-1851.	1.7	24
88	Structures, spectra, and electronic properties of halide-water pentamers and hexamers, Xâ^'(H2O)5,6 (X=F,Cl,Br,I): Ab initio study. Journal of Chemical Physics, 2002, 116, 5509-5520.	1.2	135
89	An Electrochemically Controllable Nanomechanical Molecular System Utilizing Edge-to-Face and Face-to-Face Aromatic Interactions. Organic Letters, 2002, 4, 3971-3974.	2.4	56