Eunji Sim

List of Publications by Year
in descending order

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90 papers	2,812 citations	159585 30 h-index	182427 51 g-index
91 all docs	91 docs citations	91 times ranked	2829 citing authors

#	Article	IF	Citations
1	Understanding and Reducing Errors in Density Functional Calculations. Physical Review Letters, 2013, 111, 073003.	7.8	271
2	Ultrathin Zirconium Disulfide Nanodiscs. Journal of the American Chemical Society, 2011, 133, 7636-7639.	13.7	149
3	Compositionâ€Dependent Hot Carrier Relaxation Dynamics in Cesium Lead Halide (CsPbX₃,) Tj ETQq1 1 0.784314 rgBT	13.8	141
4	Filtered propagator functional for iterative dynamics of quantum dissipative systems. Computer Physics Communications, 1997, 99, 335-354.	7.5	98
5	Long-time quantum simulation of the primary charge separation in bacterial photosynthesis.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 3926-3931.	7.1	97
6	Communication: Avoiding unbound anions in density functional calculations. Journal of Chemical Physics, 2011, 134, 171103.	3.0	93
7	The Importance of Being Inconsistent. Annual Review of Physical Chemistry, 2017, 68, 555-581.	10.8	93
8	Path Integral Simulation of Charge Transfer Dynamics in Photosynthetic Reaction Centers. Journal of Physical Chemistry B, 1997, 101, 5446-5458.	2.6	89
9	Ions in solution: Density corrected density functional theory (DC-DFT). Journal of Chemical Physics, 2014, 140, 18A528.	3.0	87
10	Quantum dynamics for a system coupled to slow baths: On-the-fly filtered propagator method. Journal of Chemical Physics, 2001, 115, 4450-4456.	3.0	83
11	Improved DFT Potential Energy Surfaces via Improved Densities. Journal of Physical Chemistry Letters, 2015, 6, 3802-3807.	4.6	79
12	Reversible Transformation of Helical Coils and Straight Rods in Cylindrical Assembly of Elliptical Macrocycles. Journal of the American Chemical Society, 2009, 131, 17768-17770.	13.7	78
13	Benchmarks and Reliable DFT Results for Spin Gaps of Small Ligand Fe(II) Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2304-2311.	5.3	71
14	Biased Helical Folding of Chiral Oligoindole Foldamers. Organic Letters, 2008, 10, 5373-5376.	4.6	70
15	Tensor propagator with weight-selected paths for quantum dissipative dynamics with long-memory kernels. Chemical Physics Letters, 1996, 249, 224-230.	2.6	67
16	Quantifying Density Errors in DFT. Journal of Physical Chemistry Letters, 2018, 9, 6385-6392.	4.6	67
17	Density Functional Analysis: The Theory of Density-Corrected DFT. Journal of Chemical Theory and Computation, 2019, 15, 6636-6646.	5.3	66
18	Ion Specificity on Electric Energy Generated by Flowing Water Droplets. Angewandte Chemie - International Edition, 2018, 57, 2091-2095.	13.8	58

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19	Identification of Droplet-Flow-Induced Electric Energy on Electrolyteâ€“Insulatorâ€“Semiconductor Structure. Journal of the American Chemical Society, 2017, 139, 10968-10971.	13.7	56
20	Quantum Rate Constants from Short-Time Dynamics:Â An Analytic Continuation Approachâ€. Journal of Physical Chemistry A, 2001, 105, 2824-2833.	2.5	50
21	Quantum time correlation functions from complex time Monte Carlo simulations: A maximum entropy approach. Journal of Chemical Physics, 2001, 114, 1075-1088.	3.0	48
22	Improving Results by Improving Densities: Density-Corrected Density Functional Theory. Journal of the American Chemical Society, 2022, 144, 6625-6639.	13.7	45
23	Timeâ€dependent discrete variable representations for quantum wave packet propagation. Journal of Chemical Physics, 1995, 102, 5616-5625.	3.0	43
24	Halogen and Chalcogen Binding Dominated by Density-Driven Errors. Journal of Physical Chemistry Letters, 2019, 10, 295-301.	4.6	43
25	Testing the kinetic energy functional: Kinetic energy density as a density functional. Journal of Chemical Physics, 2003, 118, 8140-8148.	3.0	38
26	Folding of Coordination Polymers into Doubleâ€Stranded Helical Organization. Chemistry - A European Journal, 2008, 14, 3883-3888.	3.3	35
27	Effect of Conformational Heterogeneity on Excitation Energy Transfer Efficiency in Directlymesoâ^'mesoLinked Zn(II) Porphyrin Arrays. Journal of Physical Chemistry B, 2005, 109, 11223-11230.	2.6	33
28	Density-Corrected DFT Explained: Questions and Answers. Journal of Chemical Theory and Computation, 2022, 18, 817-827.	5.3	33
29	Excitedâ€State Dynamic Planarization of Cyclic Oligothiophenes in the Vicinity of a Ringâ€toâ€Linear Excitonic Behavioral Turning Point. Angewandte Chemie - International Edition, 2015, 54, 12711-12715.	13.8	32
30	On the Bayesian approach to calculating time correlation functions in quantum systems; reaction dynamics and spectroscopy. Chemical Physics, 2001, 268, 21-34.	1.9	30
31	Pore dilatation increases the bicarbonate permeability of CFTR, ANO1 and glycine receptor anion channels. Journal of Physiology, 2016, 594, 2929-2955.	2.9	30
32	Compositionâ€Dependent Hot Carrier Relaxation Dynamics in Cesium Lead Halide (CsPbX₃,) Tj ETQq0 0 0 rgBT /Overlock 1	2.0	29
33	Density Sensitivity of Empirical Functionals. Journal of Physical Chemistry Letters, 2021, 12, 800-807.	4.6	29
34	Measuring Density-Driven Errors Using Kohnâ€“Sham Inversion. Journal of Chemical Theory and Computation, 2020, 16, 5014-5023.	5.3	28
35	Superatomâ€inâ€Superatom [RhH@Ag₂₄(SPhMe₂)₁₈]^{2â^'} Nanocluster. Angewandte Chemie - International Edition, 2021, 60, 22293-22300.	13.8	28
36	Plasmon-enhanced total-internal-reflection fluorescence by momentum-mismatched surface nanostructures. Optics Letters, 2009, 34, 3905.	3.3	23

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37	Explaining and Fixing DFT Failures for Torsional Barriers. Journal of Physical Chemistry Letters, 2021, 12, 2796-2804.	4.6	23
38	Stepped Strips from Self-Organization of Oligo(p-phenylene) Rods with Lateral Dendritic Chains. Journal of the American Chemical Society, 2008, 130, 14448-14449.	13.7	22
39	Nonmonotonic Size-Dependent Carrier Mobility in PbSe Nanocrystal Arrays. Journal of Physical Chemistry Letters, 2012, 3, 714-719.	4.6	22
40	Segmented coupled-wave analysis of a curved wire-grid polarizer. Journal of the Optical Society of America A: Optics and Image Science, and Vision, 2008, 25, 558.	1.5	20
41	Modulation of the photoelectrochemical behavior of Au nanoclusterâ€“TiO2 electrode by doping. Chemical Science, 2020, 11, 6248-6255.	7.4	20
42	Molecular Dipole Chains II. Journal of Physical Chemistry B, 1999, 103, 8663-8670.	2.6	18
43	Determination of the Electron Transfer Mechanism through Decomposition of the Density Matrix. Journal of Physical Chemistry B, 2004, 108, 19093-19095.	2.6	16
44	The Role of Linkers in the Excited-State Dynamic Planarization Processes of Macrocyclic Oligothiophene 12-Mers. Journal of Physical Chemistry Letters, 2015, 6, 4444-4450.	4.6	15
45	KS-pies: Kohnâ€“Sham inversion toolkit. Journal of Chemical Physics, 2021, 154, 124122.	3.0	15
46	Blazed wire-grid polarizer for plasmon-enhanced polarization extinction: design and analysis. Optics Express, 2017, 25, 8098.	3.4	14
47	A New Semiempirical Approach to Study Ground and Excited States of Metal Complexes in Biological Systemsâ€. Journal of Physical Chemistry B, 2002, 106, 8038-8046.	2.6	13
48	Influence of the block hydrophilicity of AB2 miktoarm star copolymers on cluster formation in solutions. Journal of Chemical Physics, 2011, 134, 204901.	3.0	13
49	Microscale heat transfer and thermal extinction of a wire-grid polarizer. Scientific Reports, 2018, 8, 14973.	3.3	13
50	Interior-filled self-assemblies of tyrosyl bolaamphiphiles regulated by hydrogen bonds. Physical Chemistry Chemical Physics, 2017, 19, 10274-10281.	2.8	12
51	Distance Dependent Coherence Variation in DNA Charge-Transfer Processes. Journal of Physical Chemistry B, 2008, 112, 2557-2561.	2.6	11
52	Effect of the Donorâ^'Bridge Energy Gap on the Electron-Transfer Mechanism in Donorâ^'Bridgeâ^'Acceptor Systems. Journal of Physical Chemistry B, 2005, 109, 11829-11835.	2.6	10
53	Ultrafast Carrierâ€“Lattice Interactions and Interlayer Modulations of Bi₂Se₃ by X-ray Free-Electron Laser Diffraction. Nano Letters, 2021, 21, 8554-8562.	9.1	10
54	Environmental Effect on the Relative Contribution of the Charge-Transfer Mechanisms within a Short DNA Sequence. Journal of Physical Chemistry B, 2006, 110, 631-636.	2.6	9

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55	Monte Carlo study of coherent diffuse photon transport in a homogeneous turbid medium: a degree-of-coherence based approach. Applied Optics, 2008, 47, 336.	2.1	9
56	Parametrization of an anharmonic Kirkwoodâ€“Keating potential for AlxGa1â^'xAs alloys. Journal of Chemical Physics, 2005, 122, 174702.	3.0	8
57	Characterization of Quantum Dynamically Significant Paths of Bridge-Mediated Charge Transfer Systems. Journal of Physical Chemistry B, 2006, 110, 13642-13648.	2.6	8
58	Evaluation of photoluminescence quenching for assessing the binding of nitroaromatic compounds to a tyrosyl bolaamphiphile self-assembly. Analyst, The, 2015, 140, 5354-5360.	3.5	8
59	Formation of Tubular Scrolls with Controlled Internal Cavity. Journal of Physical Chemistry B, 2012, 116, 1796-1801.	2.6	7
60	Superatomâ€inâ€Superatom [RhH@Ag₂₄(SPhMe₂)₁₈]^{2â^'} Nanocluster. Angewandte Chemie, 2021, 133, 22467-22474.	2.0	7
61	Surface Graft Configuration Dependency of the Morphologies of Heterosurface Sheet Polymers. Journal of Physical Chemistry B, 2012, 116, 5771-5776.	2.6	6
62	Formation of Rigid Organic Nanotubes with Controlled Internal Cavity Based on Frustrated Aggregate Internal Rearrangement Mechanism. Journal of Physical Chemistry B, 2013, 117, 7763-7770.	2.6	6
63	Self-rolled nanotubes with controlled hollow interiors by patterned grafts. Soft Matter, 2015, 11, 3714-3723.	2.7	6
64	Fluorometric detection of nitroaromatics by fluorescent lead complexes: A spectroscopic assessment of detection mechanism. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 194, 222-229.	3.9	6
65	Glass formation and local disorder: Amorphization in planar clusters. Journal of Chemical Physics, 1998, 109, 7901-7906.	3.0	5
66	Degree of Coherence of Single-Component Molecular Wires: Dependence on Length, Coupling Strength, and Dissipative Medium. Journal of Physical Chemistry C, 2010, 114, 1312-1316.	3.1	5
67	Pathway Analysis on DNA Charge Transfer through Adenine and Guanine Bridges. Journal of Physical Chemistry C, 2010, 114, 20394-20400.	3.1	5
68	Supercooling in a two-dimensional Lennard-Jones mixture. Journal of Chemical Physics, 2001, 114, 9048-9058.	3.0	4
69	Analysis of Bridge-Mediated Pathways for Long-Range Charge Transfer Systems. Journal of Physical Chemistry B, 2006, 110, 16803-16807.	2.6	4
70	Distance-dependent charge transfer mechanism in adenine bridging DNA sequences. Current Applied Physics, 2009, 9, e276-e279.	2.4	4
71	Direct observation of structural properties and fluorescent trapping sites in macrocyclic porphyrin arrays at the single-molecule level. Physical Chemistry Chemical Physics, 2016, 18, 3871-3877.	2.8	4
72	Effect of Nanogap-Based Light-Matter Colocalization on the Surface Plasmon Resonance Detection. Journal of Lightwave Technology, 2017, 35, 4721-4727.	4.6	4

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73	Ion Specificity on Electric Energy Generated by Flowing Water Droplets. Angewandte Chemie, 2018, 130, 2113-2117.	2.0	4
74	Conformational Heterogeneity in Large Macrocyclic Thiophenes. Journal of Physical Chemistry Letters, 2019, 10, 4136-4141.	4.6	4
75	Atomic classes: Rearrangement processes. Journal of Chemical Physics, 1999, 110, 6519-6529.	3.0	3
76	Coherence Length Determination of mesoâ^'meso Linked Porphyrin Arrays Based on Forwardâ^'Backward Pair Trajectory Analysis. Journal of Physical Chemistry A, 2008, 112, 5040-5045.	2.5	3
77	Investigation and Control of Single Molecular Structures of Mesoâ€“Meso Linked Long Porphyrin Arrays. Journal of Physical Chemistry B, 2018, 122, 5121-5125.	2.6	3
78	Local Structure Invariant Potential for In_xGa_{1-x}As Semiconductor Alloys. Bulletin of the Korean Chemical Society, 2009, 30, 857-862.	1.9	2
79	Computation of Electron Delocalization for Extended Cyclic Conjugated Molecules. Australian Journal of Chemistry, 2016, 69, 999.	0.9	1
80	Coherent excitation energy transfer of meso-meso linked porphyrin array. , 2007, , .		0
81	Size-dependent quantum dynamical influence of metal nanoparticles on surface plasmon resonance. , 2007, 6479, 308.		0
82	Concentration dependent absorption and scattering characteristics of gold nanoparticles embedded in liquid phantoms. , 2007, , .		0
83	Size-dependent quantum dynamical perturbation of gold nanoparticles on surface plasmon resonance. , 2007, , .		0
84	Momentum mismatch for improved plasmon enhanced total internal reflection fluorescence imaging. Proceedings of SPIE, 2010, , .	0.8	0
85	Dissociation curves of diatomic molecules: A DC-DFT study. AIP Conference Proceedings, 2015, , .	0.4	0
86	Frontispiz: Superatomâ€inâ€Superatom [RhH@Ag₂₄(SPhMe₂)₁₈]^{2â^'} Nanocluster. Angewandte Chemie, 2021, 133, .	2.0	0
87	Frontispiece: Superatomâ€inâ€Superatom [RhH@Ag₂₄(SPhMe₂)₁₈]^{2â^'} Nanocluster. Angewandte Chemie - International Edition, 2021, 60, .	13.8	0
88	Thermal properties and extinction of a wire-grid polarizer. , 2019, , .		0
89	<scp>Softâ€wall</scp> ion transfer channel accurately predicts sterically hindered ion channel permeability. Bulletin of the Korean Chemical Society, 2022, 43, 514-522.	1.9	0
90	Thermal extinction and image misregistration on metallic nanowire arrays. , 2022, , .		0