Dong Wang

List of Publications by Year in Descending Order

91 papers	5,445 citations	41 h-index	73 g-index
96 ext. papers	6,377 ext. citations	7.5 avg, IF	6.01 L-index

#	Paper	IF	Citations
91	Temperature-Responsive Self-Assembly of Single Polyoxometalates Clusters Driven by Hydrogen Bonds. *Advanced Functional Materials*, **2021**, 31, 2103561	15.6	4
90	Aggregation-Induced Emission: A Rising Star in Chemistry and Materials Science. *Chinese Journal of Chemistry*, **2021**, 39, 677-689	4.9	24
89	Ferroelectricity in 2D metal phosphorus trichalcogenides and van der Waals heterostructures for photocatalytic water splitting. *Journal of Materials Chemistry A*, **2021**, 9, 2734-2741	13	8
88	Efficient fabrication of MoS2 nanocomposites by water-assisted exfoliation for nonvolatile memories. *Green Chemistry*, **2021**, 23, 3642-3648	10	8
87	Janus luminogens with bended intramolecular charge transfer: Toward molecular transistor and brain imaging. *Matter*, **2021**,	12.7	3
86	Metal-Free Magnetism in Chemically Doped Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2020**, 142, 11013-11021	16.4	15
85	Fuller-Rylenes: Cross-Dimensional Molecular Carbons. *CCS Chemistry*, **2020**, 2, 271-279	7.2	14
84	Anticancer Polymers via the Biginelli Reaction. *ACS Macro Letters*, **2020**, 9, 1249-1254	6.6	8
83	Visible-light-switched electron transfer over single porphyrin-metal atom center for highly selective electroreduction of carbon dioxide. *Nature Communications*, **2019**, 10, 3844	17.4	66
82	High-Performance Organic Thermoelectric Materials: Theoretical Insights and Computational Design. *Advanced Electronic Materials*, **2019**, 5, 1800882	6.4	24
81	Reducing Lattice Thermal Conductivity of the Thermoelectric SnSe Monolayer: Role of Phonon□lectron Coupling. *Journal of Physical Chemistry C*, **2019**, 123, 12001-12006	3.8	11
80	Boosting the Seebeck Coefficient for Organic Coordination Polymers: Role of Doping-Induced Polaron Band Formation. *Journal of Physical Chemistry Letters*, **2019**, 10, 2493-2499	6.4	9
79	Unveiling the Layer-Dependent Catalytic Activity of PtSe Atomic Crystals for the Hydrogen Evolution Reaction. *Angewandte Chemie - International Edition*, **2019**, 58, 6977-6981	16.4	50
78	Unveiling the Layer-Dependent Catalytic Activity of PtSe2 Atomic Crystals for the Hydrogen Evolution Reaction. *Angewandte Chemie*, **2019**, 131, 7051-7055	3.6	27
77	Charge control of fluorescent probes to selectively target the cell membrane or mitochondria: theoretical prediction and experimental validation. *Materials Horizons*, **2019**, 6, 2016-2023	14.4	21
76	Single molecule-mediated assembly of polyoxometalate single-cluster rings and their three-dimensional superstructures. *Science Advances*, **2019**, 5, eaax1081	14.3	35
75	Hydrogen Bonding-Induced Morphology Dependence of Long-Lived Organic Room-Temperature Phosphorescence: A Computational Study. *Journal of Physical Chemistry Letters*, **2019**, 10, 6948-6954	6.4	45

74	Pressure-induced emission enhancement in hexaphenylsilole: a computational study. *Journal of Materials Chemistry C*, **2019**, 7, 1388-1398	7.1	19
73	cis-C?C Bond and Amide Regulated Oriented Supramolecular Assembly on Two-Dimensional Atomic Crystals. *Journal of Physical Chemistry C*, **2019**, 123, 30996-31002	3.8	1
72	Continuous synthesis of carbon dots with full spectrum fluorescence and the mechanism of their multiple color emission. *Lab on A Chip*, **2019**, 19, 3974-3978	7.2	16
71	MOlecular MAterials Property Prediction Package (MOMAP) 1.0: a software package for predicting the luminescent properties and mobility of organic functional materials. *Molecular Physics*, **2018**, 116, 1078-1090	1.7	110
70	Lattice thermal conductivity of monolayer AsP from first-principles molecular dynamics. *Physical Chemistry Chemical Physics*, **2018**, 20, 14024-14030	3.6	20
69	CsPbICl, All-Inorganic Two-Dimensional Ruddlesden-Popper Mixed Halide Perovskite with Optoelectronic Response. *Journal of the American Chemical Society*, **2018**, 140, 11085-11090	16.4	110
68	Theoretical Studies on the Deformation Potential, Electron-Phonon Coupling, and Carrier Transports of Layered Systems. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2018**, 34, 961-976	3.8	13
67	Janus monolayer of WSeTe, a new structural phase transition material driven by electrostatic gating. *Nanoscale*, **2018**, 10, 21629-21633	7.7	41
66	Layer-Dependent Chemically Induced Phase Transition of Two-Dimensional MoS. *Nano Letters*, **2018**, 18, 3435-3440	11.5	50
65	Doping optimization of organic-inorganic hybrid perovskite CH3NH3PbI3 for high thermoelectric efficiency. *Synthetic Metals*, **2017**, 225, 108-114	3.6	27
64	Theoretical Study of Conversion and Decay Processes of Excited Triplet and Singlet States in a Thermally Activated Delayed Fluorescence Molecule. *Journal of Physical Chemistry C*, **2017**, 121, 13448-13456	3.8	91
63	Suppression of the Charge Density Wave State in Two-Dimensional 1T-TiSe by Atmospheric Oxidation. *Angewandte Chemie - International Edition*, **2017**, 56, 8981-8985	16.4	27
62	Kinetics-Controlled Amphiphile Self-Assembly Processes. *Journal of Physical Chemistry Letters*, **2017** , 8, 1798-1803	6.4	14
61	Supramolecular catalyst functions in catalytic amount: cucurbit[8]uril accelerates the photodimerization of Brooker merocyanine. *Chemical Science*, **2017**, 8, 8357-8361	9.4	60
60	Intrinsic Charge Transport in Stanene: Roles of Bucklings and Electron Phonon Couplings. *Advanced Electronic Materials*, **2017**, 3, 1700143	6.4	38
59	Tuning Thermal Transport in Chain-Oriented Conducting Polymers for Enhanced Thermoelectric Efficiency: A Computational Study. *Advanced Functional Materials*, **2017**, 27, 1702847	15.6	41
58	Probing the crystallographic orientation of two-dimensional atomic crystals with supramolecular self-assembly. *Nature Communications*, **2017**, 8, 377	17.4	25
57	Puckered Arsenene: A Promising Room-Temperature Thermoelectric Material from First-Principles Prediction. *Journal of Physical Chemistry C*, **2017**, 121, 19080-19086	3.8	42

56	GeAs2: A IV–V Group Two-Dimensional Semiconductor with Ultralow Thermal Conductivity and High Thermoelectric Efficiency. *Chemistry of Materials*, **2017**, 29, 6261-6268	9.6	57
55	Strain induced polymorphism and band structure modulation in low-temperature 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene single crystal. *Science China Chemistry*, **2017**, 60, 275-283	7.9	3
54	Supramolecular organic nanofibers with highly efficient and stable visible light photooxidation performance. *Applied Catalysis B: Environmental*, **2017**, 202, 289-297	21.8	124
53	Intrinsic and Extrinsic Charge Transport in CH3NH3PbI3 Perovskites Predicted from First-Principles. *Scientific Reports*, **2016**, 7, 19968	4.9	103
52	Controlled orientation of perovskite films through mixed cations toward high performance perovskite solar cells. *Nano Energy*, **2016**, 27, 87-94	17.1	102
51	High thermoelectric performance from optimization of hole-doped CuInTe2. *Physical Chemistry Chemical Physics*, **2016**, 18, 5925-31	3.6	27
50	Influence of alkyl side-chain length on the carrier mobility in organic semiconductors: herringbone vs. pi–pi stacking. *Journal of Materials Chemistry C*, **2016**, 4, 4546-4555	7.1	64
49	Indirect-to-Direct Band Gap Crossover in Few-Layer Transition Metal Dichalcogenides: A Theoretical Prediction. *Journal of Physical Chemistry C*, **2016**, 120, 21866-21870	3.8	66
48	Self-assembling 1D core/shell microrods by the introduction of additives: a one-pot and shell-tunable method. *Chemical Science*, **2015**, 6, 4907-4911	9.4	8
47	Unravelling Doping Effects on PEDOT at the Molecular Level: From Geometry to Thermoelectric Transport Properties. *Journal of the American Chemical Society*, **2015**, 137, 12929-38	16.4	129
46	Electronic properties and charge carrier mobilities of graphynes and graphdiynes from first principles. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 215-227	7.9	34
45	Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Nonradiative Decay: A Theoretical Proposal. *Journal of Physical Chemistry C*, **2015**, 119, 5040-5047	3.8	59
44	Few-quintuple Bi_2Te_3 nanofilms as potential thermoelectric materials. *Scientific Reports*, **2015**, 5, 8099	4.9	41
43	Tunable Electronic Properties of Two-Dimensional Transition Metal Dichalcogenide Alloys: A First-Principles Prediction. *Journal of Physical Chemistry Letters*, **2014**, 5, 285-91	6.4	77
42	Aggregation induced blue-shifted emission--the molecular picture from a QM/MM study. *Physical Chemistry Chemical Physics*, **2014**, 16, 5545-52	3.6	138
41	Nonadiabatic Molecular Dynamics Modeling of the Intrachain Charge Transport in Conjugated Diketopyrrolo-pyrrole Polymers. *Journal of Physical Chemistry C*, **2014**, 118, 6631-6640	3.8	26
40	Electron-phonon couplings and carrier mobility in graphynes sheet calculated using the Wannier-interpolation approach. *Journal of Chemical Physics*, **2014**, 141, 034704	3.9	52
39	Aggregation effects on the optical emission of 1,1,2,3,4,5-hexaphenylsilole (HPS): a QM/MM study. *Journal of Physical Chemistry A*, **2014**, 118, 9094-104	2.8	92

38	Systematic analysis of reactivities and fragmentation of glutathione and its isomer GluCysGly. *Journal of Physical Chemistry A*, **2014**, 118, 8222-8	2.8	5
37	Search for Organic Thermoelectric Materials with High Mobility: The Case of 2,7-Dialkyl[1]benzothieno[3,2-b][1]benzothiophene Derivatives. *Chemistry of Materials*, **2014**, 26, 2669-2677	9.6	66
36	Understanding Lattice Strain-Controlled Charge Transport in Organic Semiconductors: A Computational Study. *Advanced Functional Materials*, **2014**, 24, 5531-5540	15.6	25
35	Computational evaluation of optoelectronic properties for organic/carbon materials. *Accounts of Chemical Research*, **2014**, 47, 3301-9	24.3	54
34	Substitution effects on the electrical tranporting properties of tetrathia[22]annulene[2,1,2,1]: experimental and theoretical investigations. *Journal of Materials Chemistry C*, **2013**, 1, 5765	7.1	14
33	Tunable band gap photoluminescence from atomically thin transition-metal dichalcogenide alloys. *ACS Nano*, **2013**, 7, 4610-6	16.7	442
32	Carrier Mobility in Graphyne Should Be Even Larger than That in Graphene: A Theoretical Prediction. *Journal of Physical Chemistry Letters*, **2013**, 4, 1443-8	6.4	254
31	Coarse-grained molecular dynamics simulations of photoswitchable assembly and disassembly. *Nanoscale*, **2013**, 5, 3681-9	7.7	21
30	Anion-binding properties of π-electron deficient cavities in bis(tetraoxacalix[2]arene[2]triazine): a theoretical study. *Journal of Physical Chemistry A*, **2013**, 117, 3844-51	2.8	12
29	Stretching single polymer chains of donor-acceptor foldamers: toward the quantitative study on the extent of folding. *Langmuir*, **2013**, 29, 14438-43	4	13
28	First-Principles Predictions of Thermoelectric Figure of Merit for Organic Materials: Deformation Potential Approximation. *Journal of Chemical Theory and Computation*, **2012**, 8, 3338-47	6.4	48
27	Modeling thermoelectric transport in organic materials. *Physical Chemistry Chemical Physics*, **2012**, 14, 16505-20	3.6	75
26	Theoretical insight into the aggregation induced emission phenomena of diphenyldibenzofulvene: a nonadiabatic molecular dynamics study. *Physical Chemistry Chemical Physics*, **2012**, 14, 14207-16	3.6	49
25	Molecular dynamics simulations of the supramolecular assembly between an azobenzene-containing surfactant and β-cyclodextrin: role of photoisomerization. *Journal of Physical Chemistry B*, **2012**, 116, 823-32	3.4	40
24	First-principles prediction of charge mobility in carbon and organic nanomaterials. *Nanoscale*, **2012**, 4, 4348-69	7.7	412
23	Anisotropic Thermal Transport in Organic Molecular Crystals from Nonequilibrium Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2011**, 115, 5940-5946	3.8	39
22	An improved dynamic Monte Carlo model coupled with Poisson equation to simulate the performance of organic photovoltaic devices. *Journal of Chemical Physics*, **2011**, 134, 124102	3.9	58
21	Electronic structure and carrier mobility in graphdiyne sheet and nanoribbons: theoretical predictions. *ACS Nano*, **2011**, 5, 2593-600	16.7	697

20	Computational characterization of organic photovoltaic devices. *Theoretical Chemistry Accounts*, **2011**, 129, 291-301	1.9	37
19	Water transport and purification in nanochannels controlled by asymmetric wettability. *Small*, **2011**, 7, 2225-31	11	61
18	Device simulation of low-band gap polymer solar cells: Influence of electron-hole pair dissociation and decay rates on open-circuit voltage. *Applied Physics Letters*, **2010**, 97, 143511	3.4	17
17	Communications: A nonperturbative quantum master equation approach to charge carrier transport in organic molecular crystals. *Journal of Chemical Physics*, **2010**, 132, 081101	3.9	35
16	Pyrolytic hydrocarbon growth from cyclopentadiene. *Journal of Physical Chemistry A*, **2010**, 114, 12411-62.8		41
15	The role of acoustic phonon scattering in charge transport in organic semiconductors: a first-principles deformation-potential study. *Science in China Series B: Chemistry*, **2009**, 52, 1646-1652		53
14	Proton transport pathway in the ClC Cl-/H+ antiporter. *Biophysical Journal*, **2009**, 97, 121-31	2.9	43
13	First-principles investigation of organic semiconductors for thermoelectric applications. *Journal of Chemical Physics*, **2009**, 131, 224704	3.9	58
12	Theoretical predictions of size-dependent carrier mobility and polarity in graphene. *Journal of the American Chemical Society*, **2009**, 131, 17728-9	16.4	247
11	Formation of naphthalene, indene, and benzene from cyclopentadiene pyrolysis: a DFT study. *Journal of Physical Chemistry A*, **2006**, 110, 4719-25	2.8	76
10	Radical-molecule reactions for aromatic growth: a case study for cyclopentadienyl and acenaphthylene. *Journal of Organic Chemistry*, **2006**, 71, 8365-71	4.2	24
9	Protein structure and dynamics from single-molecule fluorescence resonance energy transfer. *Journal of Physical Chemistry B*, **2005**, 109, 1626-34	3.4	17
8	High-resolution Fourier transform spectrum of the (4000) local mode overtone of GeH 4 : local mode effect. *Journal of Molecular Structure*, **2000**, 517-518, 41-51	3.4	17
7	Coriolis interaction in the local mode (n100;F2) combination states of GeH4. *Molecular Physics*, **2000**, 98, 1409-1413	1.7	2
6	An ab initio quartic force field of PH3. *Journal of Chemical Physics*, **2000**, 112, 9624-9631	3.9	39
5	Nonlinearity of the Dipole Moment Surface and Intensities Anomaly of CHCl 3. *Chinese Physics Letters*, **2000**, 17, 13-15	1.8	7
4	High resolution spectroscopic study of CH3D in the region 5900–6100 cm−1. *Molecular Physics*, **1999**, 97, 787-795	1.7	13
3	High-Resolution Infrared Spectrum of H3SiI in the nu1/nu4 Region near 2200 cm-1. *Journal of Molecular Spectroscopy*, **1998**, 190, 240-7	1.3	4

2	High resolution vibration–rotation spectra of the arsine local mode (110 A1/E) band. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 1397-1401		5
1	Understanding the Temperature Dependence of the Seebeck Coefficient from First-Principles Band Structure Calculations for Organic Thermoelectric Materials. *CCS Chemistry*,1477-1483	7.2	4