Shiwei Yin

List of Publications by Year in Descending Order

71 papers	2,590 citations	25 h-index	50 g-index
76 ext. papers	2,823 ext. citations	4.4 avg, IF	4.8 L-index

#	Paper	IF	Citations
71	Insightful understanding of charge transfer processes in metalated phthalocyanines.. *Physical Chemistry Chemical Physics*, **2022**, 24, 7635-7641	3.6	
70	Inter-anion chalcogen bonds: Are they anti-electrostatic in nature?. *Journal of Chemical Physics*, **2021**, 155, 234302	3.9	1
69	Classical Electrostatics Remains the Driving Force for Interanion Hydrogen and Halogen Bonding. *Journal of Physical Chemistry A*, **2021**, 125, 10428-10438	2.8	1
68	The effect of asymmetric external reorganization energy on electron and hole transport in organic semiconductors. *Physical Chemistry Chemical Physics*, **2021**, 23, 15236-15244	3.6	1
67	Energetic molecule specific polarizable force field. *FirePhysChem*, **2021**, 1, 179-179		1
66	Multiscale Modeling of Charge Transfer Processes in Organic Semiconductors **2021**, 1-28		
65	N,F-Codoped Carbon Nanocages: An Efficient Electrocatalyst for Hydrogen Peroxide Electroproduction in Alkaline and Acidic Solutions. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 2883-2891	8.3	30
64	Stereoselective Synthesis of ()-3-Alkylideneoxindoles Gold(I)-Catalyzed Cross-Coupling of 3-Diazooxindoles with Diazoesters. *Journal of Organic Chemistry*, **2020**, 85, 5863-5871	4.2	5
63	Resonance-assisted/impaired anion-interaction: towards the design of novel anion receptors.. *RSC Advances*, **2020**, 10, 36181-36191	3.7	3
62	Theoretical Understanding of Electrocatalytic Hydrogen Production Performance by Low-Dimensional Metal-Organic Frameworks on the Basis of Resonant Charge-Transfer Mechanisms. *Journal of Physical Chemistry Letters*, **2019**, 10, 6955-6961	6.4	4
61	State-specific electrostatic potential descriptors for estimating solvatochromic effects. *Journal of Molecular Modeling*, **2019**, 25, 60	2	2
60	A fragment-based approach to evaluate the performance of AMOEBA polarizable force field on charge-carrier electronic polarization. *Chemical Physics*, **2019**, 516, 84-91	2.3	2
59	Gold(I)-Catalyzed Synthesis of Six-Membered P,O-Heterocycles via Hydration/Intramolecular Cyclization Cascade Reaction. *Advanced Synthesis and Catalysis*, **2019**, 361, 4227-4231	5.6	2
58	Salt-Templated Construction of Ultrathin Cobalt Doped Iron Thiophosphite Nanosheets toward Electrochemical Ammonia Synthesis. *Small*, **2019**, 15, e1903500	11	36
57	Synergistic Nanotubular Copper-Doped Nickel Catalysts for Hydrogen Evolution Reactions. *Small*, **2018**, 14, e1704137	11	77
56	DFT-derived atomic multipoles in AMOEBA force field for calculating intermolecular interactions of azabenzenes dimers. *Computational and Theoretical Chemistry*, **2018**, 1132, 35-41	2	3
55	Chalcogen atom modulated persistent room-temperature phosphorescence through intramolecular electronic coupling. *Chemical Communications*, **2018**, 54, 9226-9229	5.8	51

54	Theoretical estimation of the dissociation energy of CT states at the acenes/C60 interfaces using fragmental-based ALMO method. *Computational and Theoretical Chemistry*, **2018**, 1140, 32-37	2	2
53	Electrostatic Polarization Energies of Charge Carriers in Organic Molecular Crystals: A Comparative Study with Explicit State-Specific Atomic Polarizability Based AMOEBA Force Field and Implicit Solvent Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 3728-3739	6.4	11
52	First-Principles Determination of Active Sites of Ni Metal-Based Electrocatalysts for Hydrogen Evolution Reaction. *ACS Applied Materials & Interfaces*, **2018**, 10, 39624-39630	9.5	23
51	Explicit Method To Evaluate the External Reorganization Energy of Charge-Transfer Reactions in Oligoacene Crystals Using the State-Specific Polarizable Force Field. *Journal of Physical Chemistry A*, **2018**, 122, 8957-8964	2.8	8
50	Energy flow in the Photosystem I supercomplex: Comparison of approximative theories with DM-HEOM. *Chemical Physics*, **2018**, 515, 262-271	2.3	13
49	Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured 2H-/1T?-MoS2 on Graphene for Enhanced Photoresponse. *Advanced Electronic Materials*, **2017**, 3, 1700024	6.4	25
48	Evaluation of electronic polarization energy in oligoacene molecular crystals using the solvated supermolecular approach. *Physical Chemistry Chemical Physics*, **2017**, 19, 14453-14461	3.6	6
47	Reunderstanding the Fluorescent Behavior of Four-Coordinate Monoboron Complexes Containing Monoanionic Bidentate Ligands. *Journal of Physical Chemistry B*, **2017**, 121, 6189-6199	3.4	15
46	Assessment of DFT functionals for calculating intermolecular interaction of nitrogen-containing heterocyclic complexes. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	2
45	Cascade C?O/C?C/C-N Bond Formation: Metal-Free Reactions of 1,4-Diynes and 1-En-4-yn-3-ones with Isoquinoline and Quinoline N-Oxides. *Organic Letters*, **2017**, 19, 4327-4330	6.2	30
44	Organic solid fluorophores regulated by subtle structure modification: color-tunable and aggregation-induced emission. *Chemical Science*, **2017**, 8, 577-582	9.4	132
43	New solvatochromic probes: performance enhancement via regulation of excited state structures. *Physical Chemistry Chemical Physics*, **2016**, 18, 25210-25220	3.6	14
42	Theoretical investigation on exciton-dissociation and charge-recombination processes of PC61BM-PTDPPSe interface. *Journal of Molecular Modeling*, **2016**, 22, 241	2	1
41	Can the Excited State Energy of a Pyrenyl Unit Be Directly Transferred to a Perylene Bisimide Moiety?. *Journal of Physical Chemistry B*, **2016**, 120, 11961-11969	3.4	5
40	Theoretical Prediction on Photovoltaic Properties of 4Cl-BPPQ/PC61BM System via Density Functional Theory Calculations. *Chinese Journal of Chemistry*, **2016**, 34, 1143-1150	4.9	4
39	Reparameterization of 12-6 Lennard-Jones potentials based on quantum mechanism results for novel tetrahedral N4 (Td) explosives. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	3
38	In-silico design of a new energetic material1-Amino-5-nitrotetrazole with high energy and density. *Computational Materials Science*, **2016**, 112, 67-74	3.2	11
37	Theoretical Investigation on Photovoltaic Properties of the BBPQ-PC61BM System. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2016**, 32, 2503-2510	3.8	3

36	Theoretical Investigation on Photovoltaic Properties of BDT and DPP Copolymer as a Promising Organic Solar Cell. *Acta Chimica Sinica*, **2016**, 74, 251	3.3	3
35	Functionality-Oriented Derivatization of Naphthalene Diimide: A Molecular Gel Strategy-Based Fluorescent Film for Aniline Vapor Detection. *ACS Applied Materials & Interfaces*, **2016**, 8, 18584-92	9.5	60
34	Selective sensing of citrate by a supramolecular ensemble formed by a phenazine copper(I) complex and a perylene diimide derivative. *New Journal of Chemistry*, **2015**, 39, 8948-8955	3.6	3
33	Molecular stacking character and charge transport properties of tetrabenzoheptacenes derivatives: the effects of nitrogen doping and phenyl substitution. *Journal of Molecular Modeling*, **2015**, 21, 126	2	3
32	Theoretical study on the electron transport properties of chlorinated pentacene derivatives. *Computational and Theoretical Chemistry*, **2015**, 1057, 67-73	2	13
31	Theoretical investigation on charge transport parameters of two novel heterotetracenes as ambipolar organic semiconductors. *Synthetic Metals*, **2014**, 188, 146-155	3.6	13
30	Effective polarization energy of the naphthalene molecular crystal: a study on the polarizable force field. *Science China Chemistry*, **2014**, 57, 1375-1382	7.9	5
29	Supramolecular electron donor–acceptor complexes formed by perylene diimide derivative and conjugated phenazines. *New Journal of Chemistry*, **2014**, 38, 5647-5653	3.6	9
28	Theoretical investigation on the crystal structures and electron transport properties of several nitrogen-rich pentacene derivatives. *Journal of Molecular Modeling*, **2014**, 20, 2158	2	9
27	Effects of global orbital cutoff value and numerical basis set size on accuracies of theoretical atomization energies. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	18
26	Electron Correlation Effects on the Longitudinal Polarizabilities and Second Hyperpolarizabilities of Polyenes: A Finite Field Study. *International Journal of Photoenergy*, **2014**, 2014, 1-6	2.1	
25	Theoretical investigation on electronic, optical, and charge transport properties of 7,8,15,16-tetraazaterrylene and its derivatives with electron-attracting substituents. *New Journal of Chemistry*, **2013**, 37, 2925	3.6	24
24	Challenges for the Accurate Simulation of Anisotropic Charge Mobilities through Organic Molecular Crystals: The β Phase of mer-Tris(8-hydroxyquinolinato)aluminum(III) (Alq3) Crystal. *Journal of Physical Chemistry C*, **2012**, 116, 14826-14836	3.8	61
23	An ultrasensitive fluorescent sensing nanofilm for organic amines based on cholesterol-modified perylene bisimide. *Chemistry - an Asian Journal*, **2012**, 7, 1576-82	4.5	68
22	Cis- and trans-isomerization-induced transition of charge transport property in PPV oligomers. *Chemical Physics*, **2011**, 388, 69-77	2.3	4
21	A New Strategy for Designing Conjugated Polymer-Based Fluorescence Sensing Films via Introduction of Conformation Controllable Side Chains. *Macromolecules*, **2011**, 44, 703-710	5.5	29
20	Pyrene-Containing Conjugated Polymer-Based Fluorescent Films for Highly Sensitive and Selective Sensing of TNT in Aqueous Medium. *Macromolecules*, **2011**, 44, 4759-4766	5.5	160
19	Theoretical study the trap and carrier-density dependent electron mobility in pentacene ab-plane by the steady master equation. *Synthetic Metals*, **2010**, 160, 1241-1246	3.6	9

18	Theoretical Studies on the Electronic Structures and Optical Properties of Tri-aryl End-capped Terthiophene Derivatives. *Chinese Journal of Chemistry*, **2010**, 28, 1907-1914	4.9	1
17	Theoretical studies on charge transport character and optional properties of Alq3 and its difluorinated derivatives. *Synthetic Metals*, **2009**, 159, 385-390	3.6	25
16	Autophosphorylation of H2AX in a cell-specific frozen dependent way. *Cryobiology*, **2008**, 57, 175-7	2.7	10
15	Theoretical investigation on the structure and electronic properties of Alq2R (R = 8-hydroxyquinoline, OH, phenolate and phenylphenolate) and its derivatives. *Computational and Theoretical Chemistry*, **2008**, 867, 116-121		8
14	Modeling hole and electron mobilities in pentacene ab-plane. *Organic Electronics*, **2008**, 9, 852-858	3.5	49
13	Assignment of the Qy absorption spectrum of photosystem-I from Thermosynechococcus elongatus based on CAM-B3LYP calculations at the PW91-optimized protein structure. *Journal of Physical Chemistry B*, **2007**, 111, 9923-30	3.4	50
12	Intramolecular electron transfer within the substituted tetrathiafulvalene-quinone dyads: facilitated by metal ion and photomodulation in the presence of spiropyran. *Journal of the American Chemical Society*, **2007**, 129, 6839-46	16.4	91
11	First-principle band structure calculations of tris(8-hydroxyquinolinato)aluminum. *Journal of Physical Chemistry B*, **2006**, 110, 3180-4	3.4	26
10	Aggregation-enhanced luminescence and vibronic coupling of silole molecules from first principles. *Physical Review B*, **2006**, 73,	3.3	108
9	Balanced carrier transports of electrons and holes in silole-based compounds--a theoretical study. *Journal of Physical Chemistry A*, **2006**, 110, 7138-43	2.8	148
8	Effects of intermolecular interaction and molecule-electrode couplings on molecular electronic conductance. *Journal of Physical Chemistry B*, **2005**, 109, 12304-8	3.4	47
7	Structures, electronic states, photoluminescence, and carrier transport properties of 1,1-disubstituted 2,3,4,5-tetraphenylsiloles. *Journal of the American Chemical Society*, **2005**, 127, 6335-46	16.4	458
6	1,3-Dithiole-2-thione derivatives featuring an anthracene unit: new selective chemodosimeters for Hg(II) ion. *Chemical Communications*, **2005**, 2161-3	5.8	187
5	Efficient blue electroluminescent device using tetra(□haphthyl)silane as a hole-blocking material. *Applied Physics Letters*, **2005**, 87, 222115	3.4	16
4	Field Effect on the Singlet and Triplet Exciton Formation in Organic/Polymeric Light-Emitting Diodes. *Journal of Physical Chemistry B*, **2004**, 108, 9608-9613	3.4	29
3	Theoretical Investigation of the Spin-dependent Exciton Formation Rates in Polymeric Light-emitting Diodes. *Journal of the Chinese Chemical Society*, **2003**, 50, 691-702	1.5	
2	Structures, electronic states, and electroluminescent properties of a zinc(II) 2-(2-hydroxyphenyl)benzothiazolate complex. *Journal of the American Chemical Society*, **2003**, 125, 14816-24	16.4	276
1	A wuantitative structure-property relationship study of the glass transition temperature of OLED materials. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 970-7		43