

Shu-Ping Huang

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114
papers

6,407
citations

28
h-index

79
g-index

127
ext. papers

7,401
ext. citations

6.2
avg, IF

5.94
L-index

#	Paper	IF	Citations
114	Efficient blue organic light-emitting diodes employing thermally activated delayed fluorescence. <i>Nature Photonics</i> , 2014 , 8, 326-332	33.9	1704
113	Design of efficient thermally activated delayed fluorescence materials for pure blue organic light emitting diodes. <i>Journal of the American Chemical Society</i> , 2012 , 134, 14706-9	16.4	1147
112	Anthraquinone-based intramolecular charge-transfer compounds: computational molecular design, thermally activated delayed fluorescence, and highly efficient red electroluminescence. <i>Journal of the American Chemical Society</i> , 2014 , 136, 18070-81	16.4	628
111	Se ₂ (B ₂ O ₇): a new type of second-order NLO material. <i>Journal of the American Chemical Society</i> , 2006 , 128, 7750-1	16.4	315
110	Triplet Exciton Confinement in Green Organic Light-Emitting Diodes Containing Luminescent Charge-Transfer Cu(I) Complexes. <i>Advanced Functional Materials</i> , 2012 , 22, 2327-2336	15.6	253
109	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3872-7	6.4	248
108	High-efficiency deep-blue organic light-emitting diodes based on a thermally activated delayed fluorescence emitter. <i>Journal of Materials Chemistry C</i> , 2014 , 2, 421-424	7.1	230
107	Bismuth Nanoparticle@Carbon Composite Anodes for Ultralong Cycle Life and High-Rate Sodium-Ion Batteries. <i>Advanced Materials</i> , 2019 , 31, e1904771	24	118
106	Explorations of new types of second-order nonlinear optical materials in Cd(Zn)-VV-TeIV-O Systems. <i>Chemistry - A European Journal</i> , 2008 , 14, 1972-81	4.8	97
105	KMBP ₂ O ₈ (M = Sr, Ba): a new kind of noncentrosymmetry borophosphate with the three-dimensional diamond-like framework. <i>Inorganic Chemistry</i> , 2009 , 48, 6623-9	5.1	84
104	Molecule-substrate interaction channels of metal-phthalocyanines on graphene on Ni(111) surface. <i>Journal of Chemical Physics</i> , 2011 , 134, 094705	3.9	71
103	Hierarchical spheres constructed by ultrathin VS ₂ nanosheets for sodium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 3691-3696	13	53
102	Safe, Low-Cost, Fast-Kinetics and Low-Strain Inorganic-Open-Framework Anode for Potassium-Ion Batteries. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 16474-16479	16.4	49
101	MnSb ₂ S ₄ Monolayer as an Anode Material for Metal-Ion Batteries. <i>Chemistry of Materials</i> , 2018 , 30, 3208-3214	9.2	38
100	Photoinduced rearrangement of vinyl tosylates to ketosulfones. <i>Green Chemistry</i> , 2017 , 19, 3530-3534	10	37
99	DFT study of the mechanism for methane hydroxylation by soluble methane monooxygenase (sMMO): effects of oxidation state, spin state, and coordination number. <i>Dalton Transactions</i> , 2013 , 42, 1011-23	4.3	36
98	Density functional theoretical determinations of electronic and optical properties of nanowires and bulks for CdS and CdSe. <i>Applied Physics Letters</i> , 2007 , 90, 031904	3.4	36

97	First-principles modeling of nonlinear optical properties of C ₃ N ₄ polymorphs. <i>Applied Physics Letters</i> , 2006 , 89, 261117	3.4	36
96	First-principles study: size-dependent optical properties for semiconducting silicon carbide nanotubes. <i>Optics Express</i> , 2007 , 15, 10947-57	3.3	35
95	Mechanism of electrochemical lithiation of a metal-organic framework without redox-active nodes. <i>Journal of Chemical Physics</i> , 2016 , 144, 194702	3.9	34
94	Y-doped Li ₈ ZrO ₆ : A Li-Ion Battery Cathode Material with High Capacity. <i>Journal of the American Chemical Society</i> , 2015 , 137, 10992-1003	16.4	33
93	Starburst Triarylamine Donor-Based Metal-Free Photosensitizers for Photocatalytic Hydrogen Production from Water. <i>Organic Letters</i> , 2017 , 19, 1048-1051	6.2	32
92	Tuning Electronic Structures of ZnO Nanowires by Surface Functionalization: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 8861-8866	3.8	32
91	Zn[Htma][ddm]: An Interesting Three-Dimensional Chiral Nonlinear Optical-Active Zinc-Trimesate Framework. <i>Crystal Growth and Design</i> , 2010 , 10, 930-936	3.5	30
90	Hierarchical Composite of Rose-Like VS @S/N-Doped Carbon with Expanded (001) Planes for Superior Li-Ion Storage. <i>Small</i> , 2019 , 15, e1903904	11	30
89	Perylenequinonoid-Catalyzed [4 + 1] and [4 + 2] Annulations of Azoalkenes: Photocatalytic Access to 1,2,3-Thiadiazole/1,4,5,6-Tetrahydropyridazine Derivatives. <i>Journal of Organic Chemistry</i> , 2019 , 84, 7711-7721	4.2	29
88	New bithiazole-functionalized organic photosensitizers for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2013 , 96, 516-524	4.6	29
87	Theoretical calculations of structures and properties of one-dimensional silicon-based nanomaterials: Particularities and peculiarities of silicon and silicon-containing nanowires and nanotubes. <i>Coordination Chemistry Reviews</i> , 2009 , 253, 2935-2958	23.2	29
86	Sulfur-Doped Anatase TiO ₂ as an Anode for High-Performance Sodium-Ion Batteries. <i>ACS Applied Energy Materials</i> , 2019 , 2, 3791-3797	6.1	28
85	Whether Corrugated or Planar Vacancy Graphene-like Carbon Nitride (g-C ₃ N ₄) Is More Effective for Nitrogen Reduction Reaction?. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 17296-17305	3.8	27
84	Electronic properties of red and black phosphorous and their potential application as photocatalysts. <i>RSC Advances</i> , 2016 , 6, 80872-80884	3.7	27
83	Perylenequinonoid-catalyzed photoredox activation for the direct arylation of (het)arenes with sunlight. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 4364-4369	3.9	26
82	Rational Design of Hierarchical SnS ₂ Microspheres with S Vacancy for Enhanced Sodium Storage Performance. <i>ACS Sustainable Chemistry and Engineering</i> , 2020 , 8, 9519-9525	8.3	26
81	Reversible conversion reaction of GeO ₂ boosts lithium-ion storage via Fe doping. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 4574-4580	13	25
80	Density Functional Theory Study of Single-Atom V, Nb, and Ta Catalysts on Graphene and Carbon Nitride for Selective Nitrogen Reduction. <i>ACS Applied Nano Materials</i> , 2020 , 3, 5149-5159	5.6	25

79	Charge Transfer, Luminescence, and Phonon Bottleneck in TiO ₂ Nanowires Computed by Eigenvectors of Liouville Superoperator. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3996-4005	6.4	23
78	A theoretical investigation of hyperpolarizability for small Ga(n)As(m) (n + m = 4-10) clusters. <i>Journal of Chemical Physics</i> , 2006 , 124, 94302	3.9	23
77	Nanocomposite of Mo ₂ N Quantum [email[protected]]@Nitrogen-Doped Carbon as a High-Performance Anode for Lithium-Ion Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 10198-10206	8.3	22
76	Excited State Dynamics of Ru ₁₀ Cluster Interfacing Anatase TiO ₂ (101) Surface and Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 2823-9	6.4	22
75	SOS TDDFT study on the dynamic third-order nonlinear optical properties of aniline oligomers based on the optimized configurations. <i>Polymer</i> , 2006 , 47, 1749-1754	3.9	22
74	Cercosporin-bioinspired selective photooxidation reactions under mild conditions. <i>Green Chemistry</i> , 2019 , 21, 6073-6081	10	21
73	Transition-Metal-Doped M-Li ₈ ZrO ₆ (M = Mn, Fe, Co, Ni, Cu, Ce) as High-Specific-Capacity Li-Ion Battery Cathode Materials: Synthesis, Electrochemistry, and Quantum Mechanical Characterization. <i>Chemistry of Materials</i> , 2016 , 28, 746-755	9.6	21
72	Synthesis, structure, and photophysics of copper(i) triphenylphosphine complexes with functionalized 3-(2-N-pyrimidinyl)-1,2,4-triazole ligands. <i>Dalton Transactions</i> , 2017 , 46, 13077-13087	4.3	21
71	Panchromatic Sensitization with Zn Porphyrin-Based Photosensitizers for Light-Driven Hydrogen Production. <i>ChemSusChem</i> , 2018 , 11, 2517-2528	8.3	20
70	Phthalocyanine and Metal Phthalocyanines Adsorbed on Graphene: A Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 16614-16620	3.8	19
69	Non-collinear spin DFT for lanthanide ions in doped hexagonal NaYF ₄ . <i>Molecular Physics</i> , 2014 , 112, 546-556	5.6	18
68	Metal-organic framework-derived hollow structure CoS/nitrogen-doped carbon spheres for high-performance lithium/sodium ion batteries. <i>Chemical Communications</i> , 2020 , 56, 3951-3954	5.8	16
67	Different Atomic Terminations Affect the Photocatalytic Nitrogen Fixation of Bismuth Oxybromide: A First Principles Study. <i>Chemistry - an Asian Journal</i> , 2018 , 13, 799-808	4.5	16
66	Electronic structure and hot carrier relaxation in <001> anatase TiO ₂ nanowire. <i>Molecular Physics</i> , 2014 , 112, 539-545	1.7	16
65	From molecule to bulk material: optical properties of hydrogen-bonded dimers [C ₁₂ H ₁₂ N ₄ O ₂ AgPF ₆] ₂ and [C ₂₈ H ₂₈ N ₆ O ₃ AgPF ₆] ₂ depend on the arrangement of the oxime moieties. <i>Chemistry - A European Journal</i> , 2007 , 13, 5151-9	4.8	16
64	Large-scale preparation of heterometallic chalcogenide MnSbS monolayer nanosheets with a high visible-light photocatalytic activity for H ₂ evolution. <i>Chemical Communications</i> , 2016 , 52, 13381-13384	5.8	15
63	Computational prediction for oxidation and reduction potentials of organic molecules used in organic light-emitting diodes. <i>Organic Electronics</i> , 2019 , 64, 216-222	3.5	15
62	Indium selenide monolayer: a two-dimensional material with strong second harmonic generation. <i>CrystEngComm</i> , 2018 , 20, 2573-2582	3.3	14

- 61 Crystal and band structure of $K_2AlTi(PO_4)_3$ with the langbeinite-type structure. *Journal of Alloys and Compounds*, **2009**, 477, 795-799 5.7 14
- 60 Synthesis, crystal and band structures, and properties of a new supramolecular complex $(Hg_2As)_2(CdI_4)$. *Journal of Solid State Chemistry*, **2007**, 180, 805-811 3.3 14
- 59 What Is the Best Size of Subnanometer Copper Clusters for CO₂ Conversion to Methanol at Cu/TiO₂ Interfaces? A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2019**, 123, 24118-24132 3.8 13
- 58 Oligothiophene-bridged bis(arylene ethynylene) small molecules for solution-processible organic solar cells with high open-circuit voltage. *Chemistry - an Asian Journal*, **2013**, 8, 1892-900 4.5 13
- 57 Syntheses, crystal structures, energy bands, and optical characterizations of $Na_5Ln(MoO_4)_4$ (Ln = Gd, Er). *Journal of Molecular Structure*, **2009**, 919, 178-184 3.4 13
- 56 Ab Initio Study on Thermal and Chemical Stabilities of Silicon Monoxide Clusters. *Journal of Physical Chemistry C*, **2009**, 113, 12736-12741 3.8 13
- 55 Localizing Holes as Polarons and Predicting Band Gaps, Defect Levels, and Delithiation Energies of Solid-State Materials with a Local Exchange-Correlation Functional. *Journal of Physical Chemistry C*, **2017**, 121, 23955-23963 3.8 12
- 54 Cercosporin-bioinspired photoreductive activation of aryl halides under mild conditions. *Journal of Catalysis*, **2019**, 380, 1-8 7.3 12
- 53 First-principles calculations of band structures and dynamic optical properties of CsCdBr₃ and RbCdI₃·2H₂O crystals. *Journal of Applied Physics*, **2006**, 99, 013516 2.5 12
- 52 Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. *Journal of Physical Chemistry C*, **2020**, 124, 7031-7038 3.8 11
- 51 A periodic density functional theory study on the effects of halides encapsulated in SiC nanotubes. *Journal of Chemical Physics*, **2008**, 129, 174108 3.9 11
- 50 Syntheses, crystal structures, and characterizations of $LiM(PO_3)_4$ (M = Y, Dy). *Journal of Molecular Structure*, **2008**, 892, 8-12 3.4 11
- 49 BC₂N/Graphene Heterostructure as a Promising Anode Material for Rechargeable Li-Ion Batteries by Density Functional Calculations. *Journal of Physical Chemistry C*, **2019**, 123, 30809-30818 3.8 11
- 48 Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. *Applied Surface Science*, **2021**, 563, 150269 6.7 11
- 47 Thiourea-based polyimide/RGO composite cathode: A comprehensive study of storage mechanism with alkali metal ions. *Science China Materials*, **2020**, 63, 1929-1938 7.1 10
- 46 First-principles study of the elastic and optical properties of the pseudocubic Si_3As_4 , Ge_3As_4 and Sn_3As_4 . *Journal of Physics Condensed Matter*, **2007**, 19, 496215 1.8 10
- 45 Conduction and Surface Effects in Cathode Materials: Li_8ZrO_6 and Doped Li_8ZrO_6 . *Journal of Physical Chemistry C*, **2016**, 120, 9637-9649 3.8 9
- 44 Toward an Accurate Description of Thermally Activated Delayed Fluorescence: Equal Importance of Electronic and Geometric Factors. *Journal of Physical Chemistry C*, **2019**, 123, 13869-13876 3.8 8

43	Electronic and vibrational properties of stable isomers of $(\text{SiO})_n((0, \text{E}))$ ($n = 2-7$) clusters. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 8893-900	2.8	8
42	SIZE EFFECT OF ENCASED ATOM ON ABSORPTION AND NONLINEAR OPTICAL PROPERTIES OF EMBEDDED METALLOFULLERENES $\text{M}@\text{C}_{82}$ ($\text{M} = \text{Sc}, \text{Y}, \text{La}$). <i>Journal of Theoretical and Computational Chemistry</i> , 2008 , 07, 737-749	1.8	8
41	Modeling of configurations and third-order nonlinear optical properties of methyl silsesquioxanes. <i>Journal of Chemical Physics</i> , 2005 , 122, 204709	3.9	8
40	Confined CoGe Alloy Nanoparticles in Nitrogen-Doped Carbon Nanotubes for Boosting Lithium Storage. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 46247-46253	9.5	8
39	N-Doped carbon encapsulating Bi nanoparticles derived from metal-organic frameworks for high-performance sodium-ion batteries. <i>Journal of Materials Chemistry A</i> ,	13	8
38	Why does F-doping enhance the photocatalytic water-splitting performance of mBiVO_4 ? A density functional theory study. <i>New Journal of Chemistry</i> , 2017 , 41, 1094-1102	3.6	7
37	Carbon-based dots for the electrochemical production of hydrogen peroxide. <i>Chemical Communications</i> , 2020 , 56, 7609-7612	5.8	7
36	Surface passivation-induced strong ferromagnetism of zinc oxide nanowires. <i>Chemistry - A European Journal</i> , 2010 , 16, 13072-6	4.8	7
35	Electronic origin for enhanced nonlinear optical response of complexes from tetraalkylammonium halide and carbon tetrabromide: electrostatic potentials of intermolecular donor-acceptor dyads. <i>Chemistry - A European Journal</i> , 2006 , 12, 6880-7	4.8	7
34	1T-MoS ₂ monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. <i>Applied Surface Science</i> , 2022 , 584, 152537	6.7	7
33	Exploring the potentials of TiN and TiNX ($X = \text{O}, \text{F}, \text{OH}$) monolayers as anodes for Li or non-Li ion batteries from first-principles calculations.. <i>RSC Advances</i> , 2019 , 9, 40340-40347	3.7	7
32	Tailoring the Linear and Second-Order Nonlinear Optical Responses of the Titanium-MIL-125 Metal-Organic Framework through Ligand Functionalization: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 653-664	3.8	7
31	Blue-AsP monolayer as a promising anode material for lithium- and sodium-ion batteries: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 5143-5151	3.6	7
30	Effects of doping high-valence transition metal (V, Nb and Zr) ions on the structure and electrochemical performance of LIB cathode material LiNiCoMnO . <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 11528-11537	3.6	7
29	Theoretical study of two-photon absorption in donor-acceptor chromophores tetraalkylammonium halide/carbon tetrabromide. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 10330-5	2.8	6
28	A New Candidate in Polyanionic Compounds for a Potassium-Ion Battery Cathode: KTiOPO . <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 2721-2726	6.4	6
27	Effect of cage charges on multiphoton absorptions: first-principles study on metallofullerenes $\text{Sc}(2)\text{C}(2)@\text{C}(68)$ and $\text{Sc}(3)\text{N}@\text{C}(68)$. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 5966-71	2.8	5
26	Easily fabricated HARCP/HAp photocatalyst for efficient and fast removal of tetracycline under natural sunlight. <i>Chemical Engineering Journal</i> , 2021 , 412, 128620	14.7	5

25	Dynamics of charge at water-to-semiconductor interface: Case study of wet [0 0 1] anatase TiO ₂ nanowire. <i>Chemical Physics</i> , 2016 , 481, 184-190	2.3	5
24	Anionic Oxygen Redox in the High-Lithium Material Li ₈ SnO ₆ . <i>Chemistry of Materials</i> , 2021 , 33, 834-844	9.6	5
23	Graphene-enhanced intermolecular interaction at interface between copper- and cobalt-phthalocyanines. <i>Journal of Chemical Physics</i> , 2015 , 143, 134706	3.9	4
22	Ab initio characterization of the electronic and optical properties of a new IR nonlinear optical crystal: K ₃ V ₅ O ₁₄ . <i>Journal of Physics Condensed Matter</i> , 2006 , 18, 5535-5544	1.8	4
21	Defective BC ₂ N as an Anode Material with Improved Performance for Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 4946-4954	3.8	4
20	UiO-66 Metal-Organic Framework as an Anode for a Potassium-Ion Battery: Quantum Mechanical Analysis. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 9679-9687	3.8	4
19	Development of Strong Visible-Light-Absorbing Cyclometalated Iridium(III) Complexes for Robust and Efficient Light - Driven Hydrogen Production.. <i>Chemistry - A European Journal</i> , 2022 ,	4.8	4
18	Anatase TiO ₂ Nanowires, Thin Films, and Surfaces: Ab initio Studies of Electronic Properties and Non-adiabatic Excited State Dynamics. <i>Materials Research Society Symposia Proceedings</i> , 2014 , 1659, 129-134		3
17	Possible Reaction Paths of Small Silicon Clusters with Oxygen Explored with Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 13196-13203	3.8	3
16	Band-gap control optical Kerr effect and light self-focusing of semiconducting materials CdxHg _{1-x} Ga ₂ S ₄ . <i>Applied Physics Letters</i> , 2005 , 87, 141905	3.4	3
15	Understanding the Role of Various Dopant Metals (Sb, Sn, Ga, Ge, and V) in the Structural and Electrochemical Performances of LiNi _{0.5} Co _{0.2} Mn _{0.3} O ₂ . <i>Journal of Physical Chemistry C</i> , 2021 , 125, 19600-19608	3.8	3
14	Carborane bridged ferrocenyl conjugated molecules: synthesis, structure, electrochemistry and photophysical properties. <i>New Journal of Chemistry</i> , 2020 , 44, 7569-7576	3.6	2
13	First-principles determinations and investigations of the electronic absorption and third-order polarizability spectra of electron donor-acceptor chromophores tetraalkylammonium halide/carbon tetrabromide. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 9249-54	2.8	2
12	Length dependence of linear and nonlinear optical properties of finite-length BN(5,0) nanotube. <i>Chinese Physics B</i> , 2006 , 15, 1563-1569		2
11	Self-Optimizing Effect in Lithium Storage of GeO Induced by Heterointerface Regulation. <i>Small</i> , 2021 , e2106067	11	2
10	Discovery and characterization of a novel perylenephotoreductant for the activation of aryl halides. <i>Journal of Catalysis</i> , 2021 , 399, 111-120	7.3	2
9	Effective Electrochemical Charge Storage in the High-Lithium Compound Li ₈ ZrO ₆ . <i>ACS Applied Energy Materials</i> , 2019 , 2, 1274-1287	6.1	1
8	Theoretical Design of Layered AlGaS ₃ as a New Nonlinear Optical Material with a Strong Second Harmonic Generation Response. <i>Crystal Growth and Design</i> , 2019 , 19, 1632-1639	3.5	1

7	Theoretical insights into the thermal reduction of N to NH over a single metal atom incorporated nitrogen-doped graphene. <i>Journal of Chemical Physics</i> , 2021 , 154, 054703	3.9	1
6	Potassium Storage Performance of UiO-66 Derivatives from First Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 4286-4295	3.8	1
5	Energy-Transfer-Mediated Photocatalysis by a Bioinspired Organic Perylenephotosensitizer HiBRCP. <i>Journal of Organic Chemistry</i> , 2021 , 86, 15284-15297	4.2	0
4	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO Activation. <i>ACS Omega</i> , 2021 , 6, 27259-27270	3.9	0
3	Validation of Density Functional Theory Methods for Predicting the Optical Properties of Cu-Based Multinary Chalcogenide Semiconductors. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 4684-4697	3.8	0
2	Investigation of Ordered TiMC and TiMCT ₂ (M = Cr and Mo; T = O and S) MXenes as High-Performance Anode Materials for Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 5283-5291	3.8	0
1	Electronic Structure and Excited State Dynamics of TiO ₂ Nanowires. <i>ACS Symposium Series</i> , 2019 , 23-46	0.4	