

Yuanzuo Li

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/1691710/yuanzuo-li-publications-by-year.pdf>

Version: 2024-04-20

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

208
papers

3,587
citations

29
h-index

54
g-index

218
ext. papers

4,072
ext. citations

3.5
avg, IF

5.71
L-index

#	Paper	IF	Citations
208	Porous Au/EAIOOH Nanoflowers for Surface-Enhanced Raman Scattering Detection of Aromatic Acid Compounds. <i>ACS Applied Nano Materials</i> , 2022 , 5, 852-861	5.6	0
207	Charge transfer processes via tandem modification of efficient non-fullerene acceptors for organic solar cells. <i>Solar Energy</i> , 2022 , 231, 503-515	6.8	2
206	Comparison of the excited-state proton transfer and single electron transfer mechanisms of the natural antioxidant Juglone and its dimer 3,3'-bijuglone. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022 , 427, 113825	4.7	0
205	Enhanced ultraviolet upconversion emission in Ho ³⁺ /Yb ³⁺ -codoped NaYF ₄ microcrystals induced by tridoping with Gd ³⁺ ions. <i>Journal of Luminescence</i> , 2022 , 243, 118619	3.8	
204	An ultrasensitive surface-enhanced Raman scattering sensor for the detection of hydrazine via the Schiff base reaction. <i>Journal of Hazardous Materials</i> , 2022 , 424, 127303	12.8	7
203	Super-Exchange Charge Transfer in One-Photon and Two-Photon Absorption of Multibranched Compounds.. <i>ACS Omega</i> , 2022 , 7, 9743-9753	3.9	
202	A sensitive surface-enhanced resonance Raman scattering sensor with bifunctional negatively charged gold nanoparticles for the determination of Cr(VI).. <i>Science of the Total Environment</i> , 2022 , 154598	10.2	1
201	Novel Clarification of Surface Plasmon Coupling Reactions of Aromatic Alkynamine and Nitro Compounds.. <i>ACS Omega</i> , 2022 , 7, 1165-1172	3.9	1
200	Examples in the detection of heavy metal ions based on surface-enhanced Raman scattering spectroscopy. <i>Nanophotonics</i> , 2021 ,	6.3	2
199	Improving the antioxidant activity of natural antioxidant honokiol by introducing the amino group. <i>Journal of Molecular Modeling</i> , 2021 , 27, 350	2	1
198	Substituent effect induced the distinctive ESIPT reaction and photophysical property of N-salicylidene-5-chloroaminopyridine. <i>Journal of Molecular Structure</i> , 2021 , 131923	3.4	0
197	Unveiling the influence of atomic electronegativity on the double ESIPT processes of uralenol: A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021 , 268, 120650	4.4	0
196	Photovoltaic performance and power conversion efficiency prediction of double fence porphyrins. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 27042-27058	3.6	2
195	Electronic and photovoltaic properties of triphenylamine-based molecules with D- π -A structures. <i>Computational and Theoretical Chemistry</i> , 2021 , 1207, 113467	2	2
194	Tactfully unveiling the effect of solvent polarity on the ESIPT mechanism and photophysical property of the 3-hydroxylflavone derivative. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021 , 267, 120496	4.4	0
193	Surface Plasmon-Induced Hot Electrons as the Racemate to Regulate Ionization. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 757-764	3.8	1
192	Universal and simple MoO ₃ substrate for identification of SERS enhancement mechanism. <i>Journal of Raman Spectroscopy</i> , 2021 , 52, 1275-1280	2.3	2

191	Significant Improvements of Near-IR Absorption, Electron Injection, and Oxidized Regeneration on Organic Sensitizers for Solar Cells. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 13109-13122	3.8	7
190	Physical Mechanism of Photoinduced Charge Transfer in One- and Two-Photon Absorption in D-D- π A Systems. <i>Materials</i> , 2021 , 14,	3.5	1
189	Theoretical study on the ESIPT processes and fluorescence properties of 2-(1H-Benzimidazol-2-yl)phenol-based derivatives. <i>Journal of Molecular Structure</i> , 2021 , 1236, 130370	3.4	3
188	Enhancement of one- and two-photon absorption and visualization of intramolecular charge transfer of pyrenyl-contained derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021 , 245, 118897	4.4	16
187	How graphene strengthened molecular photoelectric performance of solar cells: A photo current-voltage assessment. <i>Solar Energy</i> , 2021 , 213, 271-283	6.8	5
186	How the functional group substitution and solvent effects affect the antioxidant activity of (+)-catechin?. <i>Journal of Molecular Liquids</i> , 2021 , 327, 114818	6	7
185	Effect of Polymerization on the Charge-Transfer Mechanism in the One (Two)-Photon Absorption Process of D-A-Type Triphenylamine Derivatives. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 777-794	2.8	1
184	Ag-ZnO Nanocomposites Are Used for SERS Substrates and Promote the Coupling Reaction of PATP. <i>Materials</i> , 2021 , 14,	3.5	2
183	Dual-spectroscopic real-time monitoring of the reduction reaction between aristolochic acid I and Fe ²⁺ and its bio-application. <i>Journal of Physical Organic Chemistry</i> , 2021 , 34, e4194	2.1	1
182	Tuning fluorescence behavior and ESIPT reaction of 2-(2-Hydroxy-phenyl)-4(3H)-quinazolinone by introducing different groups. <i>Journal of Luminescence</i> , 2021 , 235, 118059	3.8	8
181	Theoretical study on the sensing mechanism of chalcone-based fluorescence probe for detecting hydrogen sulfide and biothiols. <i>New Journal of Chemistry</i> , 2021 , 45, 16906-16912	3.6	3
180	One-Step Synthesis of Gold Nanoparticles Using Liquid Crystal Molecules for Surface-Enhanced Raman Scattering Detection. <i>Plasmonics</i> , 2020 , 15, 1675-1681	2.4	
179	First-principles prediction of structural, mechanical and thermal properties of perovskite BaZrS ₃ . <i>European Physical Journal B</i> , 2020 , 93, 1	1.2	2
178	Enhancing Charge Transfer and Photoelectric Characteristics for Organic Solar Cells. <i>Journal of Nanomaterials</i> , 2020 , 2020, 1-12	3.2	
177	Effect of graphene between photoanode and sensitizer on the intramolecular and intermolecular electron transfer process. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 6391-6400	3.6	28
176	Screening of functional monomers and solvents for the molecular imprinting of paclitaxel separation: a theoretical study. <i>Journal of Molecular Modeling</i> , 2020 , 26, 26	2	4
175	Conversion of PATP to DMAB based on Ag ⁺ -induced catalytic oxidation. <i>Journal of Raman Spectroscopy</i> , 2020 , 51, 838-843	2.3	2
174	The Efficient Ionization Reaction of DTBA Achieved by Surface Plasmon Catalysis Effect. <i>Plasmonics</i> , 2020 , 15, 1525-1532	2.4	1

173	Enhanced photoelectric and photocatalysis performances of quinacridone derivatives by forming D-BA-A structure. <i>Solar Energy</i> , 2020 , 201, 872-883	6.8	20
172	One- and two-photon absorption properties of quadrupolar A-ED-BA dyes with donors of varying strengths. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 230, 118015	4.4	6
171	Tunable linear and nonlinear optical properties of chromophores containing 3,7-(di)vinylquinoxalinone core by modification of receptors moieties. <i>Optical Materials</i> , 2020 , 99, 109580-3	2.3	12
170	Effect of charge transport channel and interaction of IDT type dyes on photoelectric characteristics. <i>Journal of Molecular Liquids</i> , 2020 , 303, 112594	6	6
169	Efficient strategies for improving the performance of EDOT derivatives and TPA derivatives-based hole transport materials for perovskite solar cells. <i>Solar Energy</i> , 2020 , 208, 10-19	6.8	6
168	A DFT study of influence of dichloromethane solvent and electric field on light absorption and electronic properties of two Quinoxaline-based solar cells. <i>Optik</i> , 2020 , 219, 165030	2.5	3
167	A P/N type silicon semiconductor loaded with silver nanoparticles used as a SERS substrate to selectively drive the coupling reaction induced by surface plasmons. <i>Nanoscale Advances</i> , 2020 , 2, 3460-3466	5.1	2
166	Characterization and Evaluation of the Solubility and Oral Bioavailability of Rutin-Ethanolate Solvate. <i>AAPS PharmSciTech</i> , 2020 , 21, 241	3.9	3
165	Effects of defects in g-CN on excited-state charge distribution and transfer: Potential for improved photocatalysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 227, 117687-4	4.4	14
164	Effect of Reaction Conditions on the Characterization of Plasmon-Driven Surface Catalytic Reduction Reaction for Para-nitroaniline in a Liquid Condition. <i>Plasmonics</i> , 2020 , 15, 31-37	2.4	4
163	Highly efficient perovskite solar cells by tuning electronic structures of thienothiophene-based as hole transport materials. <i>Molecular Physics</i> , 2020 , 118, e1644383	1.7	
162	Global performance evaluation of solar cells using two models: from charge-transfer and recombination mechanisms to photoelectric properties. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 1934-1947	7.1	51
161	Introducing Asymmetry Induced by Benzene Substitution in a Rigid Fused Spacer of DA-Type Solar Cells: A Computational Investigation. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 4007-4021	3.8	33
160	Photoinduced charge transfer rate of Cy3/C blend material. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019 , 220, 117145	4.4	2
159	Tunable electron transfer rate in a CdSe/ZnS-based complex with different anthraquinone chloride substitutes. <i>Scientific Reports</i> , 2019 , 9, 7756	4.9	4
158	DFT Characteristics of Charge Transport in DBTP-Based Hole Transport Materials. <i>Applied Sciences (Switzerland)</i> , 2019 , 9, 2244	2.6	5
157	Modification of NFA-Conjugated Bridges with Symmetric Structures for High-Efficiency Non-Fullerene PSCs. <i>Polymers</i> , 2019 , 11,	4.5	10
156	Isomerization of ,Qdiiodoazobenzene Controlled by the Surface Plasmon-Assisted Reaction. <i>ACS Omega</i> , 2019 , 4, 7076-7081	3.9	2

155	Molecular engineering mechanism of organic photoactive layer by alkyl chains, 4-butoxyphenyl and cyanogroup. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019 , 218, 142-154	4.4	2
154	Second-Order Nonlinear Optical Switch Manipulation of Photosensitive Layer by an External Electric Field Coupled with Graphene Quantum Dots. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 7401-7407	2.8	10
153	Light Harvesting and Optical-Electronic Properties of Two Quercitin and Rutin Natural Dyes. <i>Applied Sciences (Switzerland)</i> , 2019 , 9, 2567	2.6	9
152	Effects of nitro- and amino-group on the antioxidant activity of genistein: A theoretical study. <i>Food Chemistry</i> , 2019 , 275, 339-345	8.5	29
151	Theoretical insights into the excited-state process of 4-tert-butyl-2-(5-(5-tert-butyl-2-methoxyphenyl)thiazolo[5,4-d]thiazol-2-yl)-phenol. <i>Journal of the Chinese Chemical Society</i> , 2019 , 66, 385-390	1.5	5
150	Design, Electron Transfer Process, and Opto-Electronic Property of Solar Cell Using Triphenylamine-Based D- π -A Architectures. <i>Materials</i> , 2019 , 12,	3.5	9
149	Photoinduced electron transfer in conjugated molecules containing different donor in an external electric field. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019 , 208, 294-298	4.4	5
148	Excited-state intramolecular proton transfer of 6-amino-2-(2'-hydroxyphenyl) benzoxazole (6A-HBO) in different solvents. <i>Journal of Physical Organic Chemistry</i> , 2019 , 32, e3901	2.1	12
147	A rigid planar low band gap polymer PTTDPP-DT-DTT for heterojunction solar cell: a study of density functional theory. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	2
146	The effect of twisted D π A configuration on electron transfer and photo-physics characteristics. <i>Molecular Physics</i> , 2018 , 116, 1179-1191	1.7	2
145	Intramolecular hydrogen bonding promoted excited state double proton transfer mechanism based on a typical molecule: Porphycene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 200, 345-350	4.4	27
144	Electron transfer and charge transport of photoelectric material in external electric field. <i>Journal of Luminescence</i> , 2018 , 199, 278-284	3.8	6
143	Electric field effect on multi-anchoring molecular architectures: Electron transfer process and opto-electronic property. <i>Journal of Molecular Liquids</i> , 2018 , 261, 123-136	6	5
142	A theoretical prediction about harnessing ESPT process for HBO derivatives. <i>Structural Chemistry</i> , 2018 , 29, 1655-1661	1.8	8
141	Characterizations of Efficient Charge Transfer and Photoelectric Performance in the Cosensitization of Solar Cells. <i>Applied Sciences (Switzerland)</i> , 2018 , 8, 1122	2.6	4
140	Plasmon-driven surface catalytic reaction of 4-ethynylaniline in a liquid environment.. <i>RSC Advances</i> , 2018 , 8, 20499-20504	3.7	1
139	Effects of the cyano substitution at different positions on the ESIPT properties of alizarin: A DFT/TD-DFT investigation. <i>Journal of Molecular Liquids</i> , 2018 , 269, 650-656	6	29
138	Experimental and Theoretical Investigation of the Photoelectrical Properties of Tetrabromophenol Blue- and Bromoxyleneol Blue-Based Solar Cells. <i>Journal of Nanomaterials</i> , 2018 , 2018, 1-13	3.2	2

137	Regulate the coupling reaction of 4-nitrothiophenol to 4,4'-dimercaptoazobenzene by organic alkali. <i>Journal of Raman Spectroscopy</i> , 2018 , 49, 1395-1401	2.3	3
136	Effects of Structural Modification on the Photoelectrical Properties of the D-A- π -A-Type Dyes in DSSCs: A Computational Investigation. <i>ChemistrySelect</i> , 2018 , 3, 6622-6637	1.8	7
135	Mechanism of surface plasmon-catalyzed reaction of fluorine phenylboronic acid. <i>Journal of Nanophotonics</i> , 2018 , 12, 1	1.1	
134	Magnetic, Mechanical, and Electronic Properties of RhH _x (x = 0, 0.25, 0.75, 1) from First-Principles Calculations. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018 , 31, 799-803	1.5	1
133	Distance-regulating surface plasmon catalyzed coupling reaction of -nitrophenyl disulfide.. <i>RSC Advances</i> , 2018 , 8, 35646-35650	3.7	2
132	A theoretical study of vibrational effects on strong field ionization of CS ₂ . <i>Journal of Theoretical and Computational Chemistry</i> , 2018 , 17, 1850052	1.8	
131	Computational Prediction of Electronic and Photovoltaic Properties of Anthracene-Based Organic Dyes for Dye-Sensitized Solar Cells. <i>International Journal of Photoenergy</i> , 2018 , 2018, 1-17	2.1	1
130	Structure and Photoelectrical Properties of Natural Photoactive Dyes for Solar Cells. <i>Applied Sciences (Switzerland)</i> , 2018 , 8, 1697	2.6	8
129	Molecular Controlling the Transport Properties for Benzothiadiazole-Based Hole Transport Materials. <i>Applied Sciences (Switzerland)</i> , 2018 , 8, 1461	2.6	1
128	A theoretical study on excited state proton transfer in 2-(2'-dihydroxyphenyl) benzoxazole. <i>Journal of Physical Organic Chemistry</i> , 2018 , 31, e3867	2.1	11
127	Physical Insight on Mechanism of Photoinduced Charge Transfer in Multipolar Photoactive Molecules. <i>Scientific Reports</i> , 2018 , 8, 10089	4.9	9
126	New Insight into the Synthesis of Aromatic Azo Compounds Assisted by Surface Plasmon Resonance. <i>Plasmonics</i> , 2017 , 12, 611-620	2.4	5
125	DFT and TD-DFT investigations of organic dye with different π -spacer used for solar cell. <i>Journal of Materials Science: Materials in Electronics</i> , 2017 , 28, 9642-9652	2.1	3
124	Screening and design of high-performance indoline-based dyes for DSSCs. <i>RSC Advances</i> , 2017 , 7, 20520-20536	3.7	30
123	A DFT Study of the Structures and Photoelectric Properties of Benzodithiophene-Based Molecules by Replacing Sulfur with a Variety of Heteroatoms (O, N, P, Si, Se). <i>ChemistrySelect</i> , 2017 , 2, 3838-3847	1.8	1
122	Vibronic quantized tunneling controlled photoinduced electron transfer in an organic solar cell subjected to an external electric field. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 16105-16112	3.6	25
121	Mechanism for the Excited-State Multiple Proton Transfer Process of Dihydroxyanthraquinone Chromophores. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 4645-4651	2.8	28
120	D π A System: Light Harvesting, Charge Transfer, and Molecular Designing. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 12546-12561	3.8	83

119	Photoactive layer based on T-shaped benzimidazole dyes used for solar cell: from photoelectric properties to molecular design. <i>Scientific Reports</i> , 2017 , 7, 45688	4.9	37
118	Tuning the Electron-Transport and Electron-Accepting Abilities of Dyes through Introduction of Different π -Conjugated Bridges and Acceptors for Dye-Sensitized Solar Cells. <i>ChemPhysChem</i> , 2017 , 18, 366-383	3.2	25
117	Theoretical and experimental study on spectra, electronic structure and photoelectric properties of three nature dyes used for solar cells. <i>Journal of Molecular Liquids</i> , 2017 , 247, 193-206	6	11
116	Double-anchoring organic dyes for dye-sensitized solar cells: the opto-electronic property and performance. <i>New Journal of Chemistry</i> , 2017 , 41, 12808-12829	3.6	8
115	A new strategy for effective distance regulation of the surface plasmon assisted coupling reaction of p-nitrothiophenol to p,p'-dimercaptoazobenzene. <i>Chemical Communications</i> , 2017 , 53, 9582-9585	5.8	12
114	Fluorescence Resonance Energy Transfer of Monomer via Photoisomerization. <i>ChemistrySelect</i> , 2017 , 2, 6446-6451	1.8	2
113	Spectral proof for the 4-aminophenyl disulfide plasma assisted catalytic reaction. <i>Scientific Reports</i> , 2017 , 7, 4358	4.9	7
112	Theoretical study on ESIPT mechanism of 2-acetyllindan-1,3-dione in hexane and acetonitrile solvents. <i>Journal of Luminescence</i> , 2017 , 183, 7-12	3.8	40
111	Insight into opto-electronic property by modifying optical layers with multi-polar and multi-branched structures. <i>Journal of Materials Science: Materials in Electronics</i> , 2017 , 28, 1489-1500	2.1	4
110	Theoretical Investigation of the ESIPT Mechanism for the 1-Hydroxy-9H-fluoren-9-one and 1-Hydroxy-11H-benzo[b]fluoren-11-one Chromophores. <i>Journal of Cluster Science</i> , 2017 , 28, 1191-1200	3	18
109	Non-Fullerene Acceptor-Based Solar Cells: From Structural Design to Interface Charge Separation and Charge Transport. <i>Polymers</i> , 2017 , 9,	4.5	18
108	Charge Distribution Dependent Spectral Analysis of the Oxidized Diferrocenyl-Oligothiophenylene-Vinylene Molecular Wires. <i>Scientific Reports</i> , 2016 , 6, 35726	4.9	2
107	Selective plasmon-driven catalysis for para-nitroaniline in aqueous environments. <i>Scientific Reports</i> , 2016 , 6, 20458	4.9	23
106	Geometries, spectra and photoelectric properties of trifluorenylamine-based photoactive layer. <i>Molecular Physics</i> , 2016 , 114, 3518-3532	1.7	1
105	Controlling light absorption and photoelectric properties of coumarin-triphenylaminedy by different acceptor functional groups. <i>Journal of Molecular Modeling</i> , 2016 , 22, 277	2	1
104	Photoinduced Electron Transfer in Organic Solar Cells. <i>Chemical Record</i> , 2016 , 16, 734-53	6.6	57
103	Optical and electrical properties of purpurin and alizarin complexone as sensitizers for dye-sensitized solar cells. <i>Journal of Materials Science: Materials in Electronics</i> , 2016 , 27, 8027-8039	2.1	16
102	Effects of different functional groups on the optical and charge transport properties of copolymers for polymer solar cells. <i>RSC Advances</i> , 2016 , 6, 61809-61820	3.7	19

101	Detailed theoretical investigation on ESIPT process of pigment yellow 101. <i>RSC Advances</i> , 2016 , 6, 59389-59394	5.7	8
100	Phase stability, elastic properties and martensitic transformation temperature of Zr ₅₀ Pd ₅₀ Ru _x alloys from first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2016 , 662, 484-488	5.7	8
99	pH-dependent plasmonic catalysis of 4-nitrobenzenethiol in aqueous environment. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 153, 542-5	4.4	6
98	Magnetic Properties, Possible Martensitic Transformation, and Elastic Properties of Heusler Alloy Fe ₂ NiSb from First-Principles Calculations. <i>Journal of Superconductivity and Novel Magnetism</i> , 2016 , 29, 1019-1024	1.5	3
97	Detailed theoretical investigation of excited-state intramolecular proton transfer mechanism of a new chromophore II. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 154, 130-134	4.4	6
96	Photoelectric Properties of DSSCs Sensitized by Phloxine B and Bromophenol Blue. <i>International Journal of Photoenergy</i> , 2016 , 2016, 1-11	2.1	4
95	An Experimental and Theoretical Investigation of the Electronic Structures and Photoelectrical Properties of Ethyl Red and Carminic Acid for DSSC Application. <i>Materials</i> , 2016 , 9,	3.5	39
94	Chemical mechanism of surface-enhanced Raman scattering via charge transfer in fluorenone-Ag complex. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 214002	1.8	6
93	Effect of the phenoxy groups on PDIB and its derivatives. <i>Scientific Reports</i> , 2016 , 6, 35555	4.9	7
92	Optical advantages of graphene on the boron nitride in visible and SW-NIR regions. <i>RSC Advances</i> , 2016 , 6, 111345-111349	3.7	13
91	Photoexcitation mechanisms of new D-π coumarin derivatives in linear and nonlinear optical processes. <i>Journal of Materials Science: Materials in Electronics</i> , 2016 , 27, 7132-7140	2.1	9
90	External electric field-dependent photoinduced electron transfer of porphyrin-bithiophene-fullerene triads. <i>Journal of Luminescence</i> , 2016 , 177, 325-330	3.8	8
89	The Charge Transfer Phenomenon in Benzene-Birene-Sulfoxide/Methanol System: Role of the Intermolecular Hydrogen Bond in Excited States. <i>Journal of Cluster Science</i> , 2015 , 26, 1463-1472	3	22
88	First-principles study of structural, elastic and electronic properties of ZrIr alloy. <i>Computational Materials Science</i> , 2015 , 105, 66-70	3.2	9
87	Study of fluorescence probe transfer mechanism based on a new type of excited-state intramolecular proton transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 144, 76-80	4.4	18
86	Insight into external electric field dependent photoinduced intermolecular charge transport in BHJ solar cell materials. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 4810-4819	7.1	54
85	Plasmon-induced dynamics of H ₂ splitting on a silver atomic chain. <i>Applied Physics Letters</i> , 2015 , 107, 083102	3.4	22
84	The excited-state multiple proton transfer mechanism of the 7-hydroxyquinoline(CH ₃ OH) ₃ cluster. <i>New Journal of Chemistry</i> , 2015 , 39, 9910-9917	3.6	34

83	A plasmon-driven selective surface catalytic reaction revealed by surface-enhanced Raman scattering in an electrochemical environment. <i>Scientific Reports</i> , 2015 , 5, 11920	4.9	41
82	Photoactive Layer of DSSCS Based on Natural Dyes: A Study of Experiment and Theory. <i>Journal of Nanomaterials</i> , 2015 , 2015, 1-6	3.2	5
81	Spectra and Charge Transport of Polar Molecular Photoactive Layers Used for Solar Cells. <i>Journal of Chemistry</i> , 2015 , 2015, 1-10	2.3	2
80	Optical Absorption and Electron Injection of 4-(Cyanomethyl)benzoic Acid Based Dyes: A DFT Study. <i>Journal of Chemistry</i> , 2015 , 2015, 1-9	2.3	2
79	Effect of aqueous and ambient atmospheric environments on plasmon-driven selective reduction reactions. <i>Scientific Reports</i> , 2015 , 5, 10269	4.9	21
78	Tunable spectra and charge transfer process of benzodifurandione-based polymer by sulfur substitution. <i>RSC Advances</i> , 2015 , 5, 18492-18500	3.7	11
77	First-Principles Study of Half-Metallic and Magnetic Properties for the Heusler Alloys Fe ₂ CrX (X = P, As, Sb, Bi). <i>Journal of Superconductivity and Novel Magnetism</i> , 2015 , 28, 1559-1564	1.5	8
76	First-Principles Study of Magnetic Properties and Martensitic Transformation of Pd [Mn In] Magnetic Shape Memory Alloys. <i>Journal of Superconductivity and Novel Magnetism</i> , 2015 , 28, 1639-1643	1.5	3
75	Fullerene-Based Photoactive Layers for Heterojunction Solar Cells: Structure, Absorption Spectra and Charge Transfer Process. <i>Materials</i> , 2014 , 8, 42-56	3.5	34
74	Theoretical study on the intramolecular charge transfer induced twisting of the nitro and dimethylamino groups. <i>Dyes and Pigments</i> , 2014 , 103, 71-75	4.6	10
73	Organic nonlinear optical materials: the mechanism of intermolecular covalent bonding interactions of Kekulé hydrocarbons with significant singlet biradical character. <i>ChemPhysChem</i> , 2014 , 15, 2626-33	3.2	4
72	Molecular design of organic sensitizers absorbing over a broadened visible region for dye-sensitized solar cells. <i>RSC Advances</i> , 2014 , 4, 57916-57922	3.7	4
71	Investigation of excited-state intramolecular proton transfer coupled charge transfer reaction of paeonol. <i>Canadian Journal of Chemistry</i> , 2014 , 92, 274-278	0.9	3
70	Theoretical Study of the Dynamic Stark Effect on Dissociation of Csl. <i>Brazilian Journal of Physics</i> , 2014 , 44, 189-193	1.2	3
69	Nonlinear optical properties and performance optimization of the pro-aromatic chromophores for NLO materials. <i>Journal of Materials Science: Materials in Electronics</i> , 2014 , 25, 5255-5263	2.1	12
68	Tip-Enhanced Raman Spectroscopy: Plasmon-Driven Selective Reductions Revealed by Tip-Enhanced Raman Spectroscopy (Adv. Mater. Interfaces 5/2014). <i>Advanced Materials Interfaces</i> , 2014 , 1, n/a-n/a	4.6	1
67	Plasmon-Driven Selective Reductions Revealed by Tip-Enhanced Raman Spectroscopy. <i>Advanced Materials Interfaces</i> , 2014 , 1, 1300125	4.6	40
66	Facile Synthesis of Micron-Sized Hollow Silver Spheres as Substrates for Surface-Enhanced Raman Scattering. <i>International Journal of Photoenergy</i> , 2014 , 2014, 1-7	2.1	2

65	Effects of hydrogen bond on 2-aminopyridine and its derivatives complexes in methanol solvent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 131, 282-7	4.4	65
64	Intermolecular hydrogen-bonding effects on photophysics and photochemistry. <i>International Reviews in Physical Chemistry</i> , 2013 , 32, 589-609	7	133
63	External Electric Field-Dependent Photoinduced Charge Transfer in a Donor-Acceptor System for an Organic Solar Cell. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 15879-15889	3.8	108
62	TDDFT studies of electronic spectra and excited states of the triphenylamine-based organic sensitizers and organic sensitizer-titanium dioxide cluster complexes. <i>RSC Advances</i> , 2013 , 3, 12133	3.7	11
61	Remote-Excitation Time-Dependent Surface Catalysis Reaction Using Plasmonic Waveguide on Sites of Single-Crystalline Crossed Nanowires. <i>Plasmonics</i> , 2013 , 8, 249-254	2.4	17
60	Nonlinear optical properties of dihydrobenzothiazolylidene and dihydroquinoinylidene compounds. <i>Optical Materials</i> , 2013 , 36, 437-443	3.3	11
59	Charge transfer and optoelectronic properties in the triarylamine-based donor-bridge-acceptor dyes for dye-sensitised solar cells. <i>Molecular Simulation</i> , 2013 , 39, 521-528	2	4
58	STRUCTURES AND SPECTROSCOPIC PROPERTIES OF THREE AROMATIC HETEROCYCLIC DYE PHOTSENSITIZERS. <i>Journal of Theoretical and Computational Chemistry</i> , 2013 , 12, 1350055	1.8	
57	Effect of electronic acceptor segments on photophysical properties of low-band-gap ambipolar polymers. <i>Scientific World Journal, The</i> , 2013 , 2013, 890215	2.2	1
56	Theoretical study of charge transfer mechanism in fullerene-phenyl-phenothiazine compound: A real-space analysis. <i>Dyes and Pigments</i> , 2012 , 92, 1344-1350	4.6	10
55	Molecular modeling of two-photon absorption and third-order nonlinearities of polymethine dyes for all-optical switching. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4141-9	2	5
54	Hydrogen-bonded Intramolecular Charge Transfer Excited State of Dimethylaminobenzophenone using Time Dependent Density Functional Theory. <i>Chinese Journal of Chemical Physics</i> , 2012 , 25, 654-658 ^{0.9}		1
53	Nonlinear resonances in electrochemical SERS of SCN ⁻ rotation-resolved Raman and anti-Stokes Raman of SCN ⁻ in HV-TERS. <i>RSC Advances</i> , 2012 , 2, 12160	3.7	2
52	Visualizations of charge transfer for the model of poly(3,4-alkylenedioxythiophene)s in neutral and various oxidation states. <i>RSC Advances</i> , 2012 , 2, 12983	3.7	8
51	A FIRST PRINCIPLE ANALYSIS ON THE STRUCTURAL AND PHOTO-INDUCED CHARGE TRANSFER IN RUTHENIUM COMPLEXES OF HEXAAZATRIPHENYLENE. <i>Journal of Theoretical and Computational Chemistry</i> , 2012 , 11, 895-905	1.8	5
50	Ab initio-based double many-body expansion potential energy surface for the first excited triplet state of the ammonia molecule. <i>Journal of Chemical Physics</i> , 2012 , 136, 194705	3.9	25
49	Time-dependent Density Functional Theory Study on the Hydrogen-bonded Dimers Formed by Gauche-1PA and Trans-1PA. <i>Journal of the Chinese Chemical Society</i> , 2012 , 59, 494-499	1.5	1
48	Direct Visual Evidence for Neutral and Charged Hexaphyrin Aromaticity with and without Keto-Defect. <i>Chinese Journal of Chemical Physics</i> , 2012 , 25, 563-570	0.9	

47	Quantum plasmonics: Symmetry-dependent plasmon-molecule coupling and quantized photoconductances. <i>Physical Review B</i> , 2012 , 86,	3.3	28
46	INTERMOLECULAR CHARGE TRANSFER ENHANCED RESONANCE RAMAN SCATTERING OF CHARGE TRANSFER COMPLEX. <i>Journal of Theoretical and Computational Chemistry</i> , 2012 , 11, 273-282	1.8	3
45	Theoretical Evidence for the Distance-Dependent Photoinduced Electron Transfer of Porphyrin-Oligothiophene-Fullerene Triads. <i>International Journal of Photoenergy</i> , 2012 , 2012, 1-10	2.1	19
44	Theoretical Characterization of the PC60BM:PDDTT Model for an Organic Solar Cell. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 21865-21873	3.8	186
43	Experimental and theoretical study of the excited state of aminostyryl terpyridine derivatives: hydrogen-bonding effects. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 81, 283-9	4.4	4
42	Theoretical study on contribution of charge transfer effect to surface-enhanced Raman scattering spectra of pyridine adsorbed on Ag(n) (n = 2-8) clusters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 82, 205-12	4.4	11
41	Time-dependent wave packet theoretical study of femtosecond photoelectron spectra and coupling between the A ₂ and B ₂ states of the NO molecule in a strong laser field. <i>Open Physics</i> , 2011 , 9,	1.3	1
40	Electrical and Raman properties of p-type and n-type modified graphene by inorganic quantum dot and organic molecule modification. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011 , 54, 416-419	3.6	14
39	Direct visualization of the charge transfer in conjugated polymers. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011 , 54, 1119-1123	3.6	1
38	Quantum mechanical study of the coupling of plasmon excitations to atomic-scale electron transport. <i>Journal of Chemical Physics</i> , 2011 , 134, 074701	3.9	80
37	STUDY OF THE S1 AND S2 EXCITED STATES OF GAS-PHASE PROTONATED SCHIFF BASE RETINAL CHROMOPHORES IN ONE AND TWO PHOTON ABSORPTION. <i>Journal of Theoretical and Computational Chemistry</i> , 2011 , 10, 121-132	1.8	2
36	THE STEREODYNAMICS STUDY OF THE C(3P) + OH (X ² Σ^-) - CO(X ¹ Σ^+) + H(2S) REACTION. <i>Journal of Theoretical and Computational Chemistry</i> , 2010 , 09, 935-943	1.8	3
35	Ascertaining p, p'-dimercaptoazobenzene Produced from p-aminothiophenol by Selective Catalytic Coupling Reaction on Silver Nanoparticles 2010 ,		2
34	Photophysical Properties of 4'-(p-aminophenyl)-2,2':6',2'-terpyridine. <i>Chinese Journal of Chemical Physics</i> , 2010 , 23, 558-564	0.9	3
33	Tunable electronic structures and optical properties of fluorenone-based molecular materials by heteroatoms. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 2230-4	2.8	20
32	Ascertaining p, p'-dimercaptoazobenzene produced from p-aminothiophenol by selective catalytic coupling reaction on silver nanoparticles. <i>Langmuir</i> , 2010 , 26, 7737-46	4	313
31	Electronic structure and optical properties of dianionic and dicationic pi-dimers. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 6972-7	2.8	28
30	Tuning the emission properties of cyclometalated platinum(II) complexes by intramolecular electron-sink/arylethynylated ligands and its application for enhanced luminescent oxygen sensing. <i>Journal of Materials Chemistry</i> , 2010 , 20, 9775		80

29	Tuning the luminescence lifetimes of ruthenium(II) polypyridine complexes and its application in luminescent oxygen sensing. <i>Journal of Materials Chemistry</i> , 2010 , 20, 1953		160
28	Local and remote charge-transfer-enhanced Raman scattering on one-dimensional transition-metal oxides. <i>Chemistry - an Asian Journal</i> , 2010 , 5, 1824-9	4.5	38
27	Tuning the Emission Colour of Triphenylamine-Capped Cyclometallated Platinum(II) Complexes and Their Application in Luminescent Oxygen Sensing and Organic Light-Emitting Diodes. <i>European Journal of Inorganic Chemistry</i> , 2010 , 2010, 4683-4696	2.3	58
26	DFT study of chemical mechanism of pre-SERS spectra in Pyrazine-metal complex and metal-Pyrazine-metal junction. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010 , 75, 794-8	4.4	14
25	Time-dependent density functional theory study on excited state intramolecular proton transfer of 3-hydroxy-2-(pyridin-2-yl)-4H-chromen-4-one. <i>Journal of Luminescence</i> , 2010 , 130, 1431-1436	3.8	14
24	Photoinduced intermolecular and intramolecular charge transfer in the mixed coaggregates of pyrazoline and dicyanonaphthalene. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009 , 205, 139-144	4.7	8
23	DFT study of adsorption site effect on surface-enhanced Raman scattering of neutral and charged pyridine-Ag ₄ complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 73, 382-7	4.4	33
22	Theoretical and experimental study on the intramolecular charge transfer excited state of the new highly fluorescent terpyridine compound. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 74, 753-7	4.4	11
21	Photo-induced charge transfer in defect-free (TiO ₂) ₁₅ nanoparticles and charge transfer from carotenoid to (TiO ₂) ₁₅ b nanoparticle in carotenoid/(TiO ₂) ₁₅ b complex used for solar cell. <i>Chemical Physics Letters</i> , 2009 , 480, 265-268	2.5	2
20	Reconsideration of the excited-state double proton transfer (ESDPT) in 2-aminopyridine/acid systems: role of the intermolecular hydrogen bonding in excited states. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 4385-90	3.6	193
19	Rational design of d-PeT phenylethynylated-carbazole monoboronic acid fluorescent sensors for the selective detection of alpha-hydroxyl carboxylic acids and monosaccharides. <i>Journal of the American Chemical Society</i> , 2009 , 131, 17452-63	16.4	215
18	Theoretical study of electronic structure and excited states properties of two dyes for dye-sensitized solar cells. <i>Molecular Physics</i> , 2009 , 107, 2569-2577	1.7	5
17	EXCITED-STATE INTRAMOLECULAR ELECTRON TRANSFER COUPLED WITH EXCITED-STATE INTRAMOLECULAR PROTON TRANSFER IN PHOTOINDUCED ENOL TO KETO TAUTOMERIZATION. <i>Journal of Theoretical and Computational Chemistry</i> , 2009 , 08, 1073-1086	1.8	
16	Density functional theory study on Herzberg-Teller contribution in Raman scattering from 4-aminothiophenol-metal complex and metal-4-aminothiophenol-metal junction. <i>Journal of Chemical Physics</i> , 2009 , 130, 234509	3.9	32
15	Photoinduced Intramolecular Charge Transfer in Donor-acceptor Dyad and Donor-bridge-acceptor Triad. <i>Chinese Journal of Chemical Physics</i> , 2008 , 21, 111-117	0.9	3
14	Intramolecular Charge Transfer of Carotene-porphyrin-fullerene Triad: Sequential or Superexchange Mechanism. <i>Chinese Journal of Chemistry</i> , 2008 , 26, 1011-1018	4.9	2
13	Intramolecular charge transfer in the dye molecules containing bis-dimethylfluoreneaniline. <i>Computational and Theoretical Chemistry</i> , 2008 , 867, 10-16		6
12	Electronic Structure and Photophysical Properties of 2-(N,N-diethylanilin-4-yl)-4,6-bis(3,5-dimethylpyrazol-1-yl)-1,3,5-triazine. <i>Chinese Journal of Chemical Physics</i> , 2007 , 20, 59-64	0.9	2

11	The effect of keto defect on the photophysical properties and electronic structure of neutral and charged LOPP. <i>Computational and Theoretical Chemistry</i> , 2007 , 803, 1-7		
10	Excited state properties of the p- and n-type semiconductors of thiazolothiazole derivative having thiophene and trifluoromethylphenyl rings. <i>Computational Materials Science</i> , 2007 , 39, 376-380	3.2	2
9	Electronic and optical properties of neutral and charged MEH-PPV. <i>Computational Materials Science</i> , 2007 , 39, 575-579	3.2	4
8	Electronic structure and optical physical properties of oligothiophenes. <i>Computational Materials Science</i> , 2007 , 39, 673-677	3.2	6
7	Excited State Properties of Fluorine-Substituted Hexabenzocoronene: A Quantum-Chemical Characterization. <i>Communications in Theoretical Physics</i> , 2006 , 46, 229-232	2.4	
6	Excited state properties of neutral, anionic and cationic 1,1-disubstituted 2,3,4,5-tetraphenylsiloles: A quantum chemical characterization. <i>Computational and Theoretical Chemistry</i> , 2006 , 770, 51-56		4
5	Intermolecular charge and energy transfer in neurosporene and chlorophyll a derivative complex. <i>Chemical Physics Letters</i> , 2005 , 412, 425-429	2.5	21
4	Intramolecular charge transfer and locally excited states of the fullerene-linked quarter-thiophenes dyad. <i>Chemical Physics Letters</i> , 2005 , 413, 110-117	2.5	30
3	Intramolecular charge transfer in the porphyrin-oligothiophene-fullerene triad. <i>Chemical Physics Letters</i> , 2005 , 416, 94-99	2.5	26
2	PCDTBT8-Doped PffBT4T-2OD-Based Ternary Solar Cells with Enhanced Open-Circuit Voltage, Fill Factor, and Charge Separation Efficiency. <i>Solar Rrl</i> , 2100670	7.1	4
1	AgNPs Functionalized with Dithizone for the Detection of Hg ²⁺ Based on Surface-enhanced Raman Scattering Spectroscopy. <i>Plasmonics</i> , 1	2.4	0