# Yu-Zhi Song

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 101 papers | 1,179 citations | 15 h-index | 29 g-index |
| 109 ext. papers | 1,526 ext. citations | 2.9 avg, IF | 4.84 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 101 | A QM/MM study on through space charge transfer-based thermally activated delayed fluorescence molecules in the solid state. *Journal of Materials Chemistry C*, **2022**, 10, 517-531 | 7.1 | 2 |
| 100 | Theoretical Study on the Light-Emitting Mechanism of Multifunctional Thermally Activated Delayed Fluorescence Molecules. *Journal of Physical Chemistry C*, **2022**, 126, 2437-2446 | 3.8 | 1 |
| 99 | Theoretical perspective of relationship between molecular structure and luminescence properties for circularly polarized thermally activated delayed fluorescence.. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2022**, 275, 121164 | 4.4 | 3 |
| 98 | Gigahertz-repetition rate, high power, ultrafast Tm-doped fiber laser source. *Optics and Laser Technology*, **2022**, 153, 108206 | 4.2 | 0 |
| 97 | Novel Deep Red Thermally Activated Delayed Fluorescence Molecule with Aggregation-Induced Emission Enhancement: Theoretical Design and Experimental Validation. *Journal of Physical Chemistry Letters*, **2022**, 13, 4711-4720 | 6.4 | 2 |
| 96 | The design of > 2000-nm, ~ 100-MHz ultrafast Tm-doped fiber soliton laser source. *Journal of Lightwave Technology*, **2021**, 1-1 | 4 | 1 |
| 95 | Field-free alignment of triatomic molecules controlled by a slow turn-on and rapid turn-off shaped laser pulse. *Molecular Physics*, **2021**, 119, e1859147 | 1.7 | 0 |
| 94 | Examining the isotope effect on CH decay and H exchange reactions: H(2S) + CH(D/T)(2). *Physica Scripta*, **2021**, 96, 015404 | 2.6 | 0 |
| 93 | Intermolecular interaction on excited-state properties of fluoro-substituted thermally activated delayed fluorescence molecules with aggregation-induced emission: a theoretical perspective. *Molecular Physics*, **2021**, 119, e1862931 | 1.7 | 1 |
| 92 | Effects of Secondary Acceptors on Excited-State Properties of Sky-Blue Thermally Activated Delayed Fluorescence Molecules: Luminescence Mechanism and Molecular Design. *Journal of Physical Chemistry A*, **2021**, 125, 175-186 | 2.8 | 3 |
| 91 | Modulation of MXene NbCT saturable absorber for passively Q-switched 2.85 μm Er:LuOlaser. *Optics Letters*, **2021**, 46, 1385-1388 | 3 | 3 |
| 90 | The Investigation on Ultrafast Pulse Formation in a Tm-Ho-Codoped Mode-Locking Fiber Oscillator. *Molecules*, **2021**, 26, | 4.8 | 2 |
| 89 | Sensing mechanism of fluorescent sensor to Cu based on inhibiting ultra-fast intramolecular proton transfer process. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 254, 119685 | 4.4 | 1 |
| 88 | Accurate High-Level -Based Global Potential Energy Surface and Quantum Dynamics Calculation for the First Excited State of CH. *Journal of Physical Chemistry A*, **2021**, 125, 5490-5498 | 2.8 | 0 |
| 87 | Investigation on the optical nonlinearity of the layered magnesium-mediated metal organic framework (Mg-MOF-74). *Optics Express*, **2021**, 29, 23786-23798 | 3.3 | |
| 86 | The theoretical study of excited-state intramolecular proton transfer of N, N,-bis (salicylidene)-(2-(3?4?-diaminophenyl) benzothiazole). *Journal of Luminescence*, **2021**, 230, 117741 | 3.8 | 14 |
| 85 | Design strategy for blue thermally activated delayed fluorescence: Position and methyl substitutions. *Chemical Physics Letters*, **2021**, 764, 138260 | 2.5 | 2 |

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| 84 | Theoretical insight into the vibrational excitation effect of the S+(4S)+H2(X1g) reaction. *Chemical Physics Letters*, **2021**, 764, 138257 | 2.5 | 0 |
| 83 | Systematic theoretical investigation of two novel molecules BtyC-1 and BtyC-2 based on ESIPT mechanism. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 258, 119810 | 4.4 | 3 |
| 82 | Broadband and enhanced nonlinear optical modulation characteristics of CuBTC for pulsed lasers. *Optical Materials Express*, **2021**, 11, 3546 | 2.6 | 1 |
| 81 | Photophysical properties of fluorescent nucleobase P-analogues expected to monitor DNA replication. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 260, 119926 | 4.4 | 2 |
| 80 | Solid-state effect on luminescent properties of thermally activated delayed fluorescence molecule with aggregation induced emission: A theoretical perspective. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 241, 118634 | 4.4 | 6 |
| 79 | A global potential energy surface for the ground electronic state of SSiH. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2020**, 53, 175203 | 1.3 | 2 |
| 78 | Investigation of excited state proton transfer mechanism for 2-(benzo[d]thiazol-2-yl)naphthalene-1,3-diol in different solvents. *Chemical Physics*, **2020**, 538, 110914 | 2.3 | 2 |
| 77 | Exploring reaction mechanism and vibrational excitation effect in H+CH(v,j=0) reaction. *Chemical Physics Letters*, **2020**, 749, 137398 | 2.5 | 1 |
| 76 | Dynamics of H(2 S) + CH(X 2) reactions based on a new CH2(${tilde{X}}^{3}A^{primeprime} $) surface via extrapolation to the complete basis set limit. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2020**, 53, 095202 | 1.3 | 2 |
| 75 | Electric Field-Modulated Surface Enhanced Raman Spectroscopy by PVDF/Ag Hybrid. *Scientific Reports*, **2020**, 10, 5269 | 4.9 | 7 |
| 74 | Mid-infrared Q-switch performance of ZrC. *Photonics Research*, **2020**, 8, 1857 | 6 | 3 |
| 73 | An investigation into self-pulsing behavior in an Er-doped ring laser. *Applied Physics Express*, **2020**, 13, 112006 | 2.4 | 0 |
| 72 | The role of intermolecular interactions in regulating the thermally activated delayed fluorescence and charge transfer properties: a theoretical perspective. *Journal of Materials Chemistry C*, **2020**, 8, 8601-8612 | 7.1 | 11 |
| 71 | Thermally activated delayed fluorescence emitters with dual conformations for white organic light-emitting diodes: mechanism and molecular design. *Physical Chemistry Chemical Physics*, **2020**, 22, 1313-1323 | 3.6 | 9 |
| 70 | Theoretical perspective for luminescent mechanism of thermally activated delayed fluorescence emitter with excited-state intramolecular proton transfer. *Journal of Materials Chemistry C*, **2020**, 8, 98-108 | 7.1 | 14 |
| 69 | Substitution effect on luminescent property of thermally activated delayed fluorescence molecule with aggregation induced emission: A QM/MM study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 229, 117964 | 4.4 | 8 |
| 68 | Suppression of aggregation caused quenching in U-shaped thermally activated delayed fluorescence molecules: Tert-butyl effect. *Journal of Luminescence*, **2020**, 219, 116899 | 3.8 | 11 |
| 67 | State-to-state dynamics of S+(2D) + H2(X1g+)(v, j) collision reaction based on the H2S+ (X 2A??)potential energy surface. *Computational and Theoretical Chemistry*, **2020**, 1191, 113021 | 2 | |

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| 66 | Theoretical Study on Thermally Activated Delayed Fluorescence Emitters in White Organic Light-Emitting Diodes: Emission Mechanism and Molecular Design. *Journal of Physical Chemistry A*, **2020**, 124, 7526-7537 | 2.8 | 4 |
| 65 | Potential energy curves, spectroscopic constants, and vibrational energy levels of CS+(X2Σ+/A2Π). *Molecular Physics*, **2020**, 118, e1597199 | 1.7 | 2 |
| 64 | The mechanism of the excited-state proton transfer of Salicylaldehyde azine and 2,2P[1,4-Phenylenebis{(E)- nitrilomethylidyne}] bisphenol: Via single or double proton transfer. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 223, 117321 | 4.4 | 6 |
| 63 | Accurate global potential energy surface for SiH (XA) and quantum dynamics of related reaction H(S) + SiH(X1Σ+). *Journal of Chemical Physics*, **2019**, 150, 224304 | 3.9 | 4 |
| 62 | The novel excited state intramolecular proton transfer broken by intermolecular hydrogen bonds in HOF system. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 219, 164-172 | 4.4 | 23 |
| 61 | Stereo-dynamics of the reaction C + SH(D,T)(v = 0, j = 0) -> H(D,T) + CS based on a recent excited state potential energy surface. *Computational and Theoretical Chemistry*, **2019**, 1155, 82-89 | 2 | 4 |
| 60 | Studies of the Coriolis coupling effect on reaction dynamics of ${rm{H}}({}^{2}{rm{S}})+{rm{O}}{{rm{H}}}^{+} rightarrow {rm{O}}({}^{3}{rm{P}})+{{rm{H}}}_{2}^{+}({{rm{{rm X}}}}^{2}{{rm{Sigma }}}_{{rm{g}}}^{+})$ using the time dependent wave packet method. *Journal of Physics B: Atomic, Molecular and Optical Physics*, | 1.3 | |
| 59 | Field-free alignment dynamics of FCN molecule induced by a terahertz half-cycle pulse. *Europhysics Letters*, **2019**, 125, 33001 | 1.6 | 6 |
| 58 | Theoretical Study on the Sensing Mechanism of Novel Hydrazine Sensor TAPHP and Its ESIPT and ICT Processes. *Frontiers in Chemistry*, **2019**, 7, 932 | 5 | 13 |
| 57 | Quantum state-to-state dynamics of O+ + H2(υ = 0, j = 0) -> OH+ (υ', j') + H reaction on a global potential energy surface. *Europhysics Letters*, **2019**, 126, 53001 | 1.6 | 5 |
| 56 | The substituent effect on the excited state intramolecular proton transfer of 3-hydroxychromone. *Chinese Physics B*, **2019**, 28, 093102 | 1.2 | 6 |
| 55 | HCS(A2A?)-based insights into the effect of vibrational excitation on the reactions C+SH (v = 0–10, j = 0) -> S+CH, H+CS. *European Physical Journal D*, **2019**, 73, 1 | 1.3 | 4 |
| 54 | Investigation on the mechanism of ESIPT of 2-hydroxy-1-naphthaldehyde-(4-pyridinecarboxylic)-hydrazone and detection of Al3+ ion. *Canadian Journal of Physics*, **2019**, 97, 721-725 | 1.1 | 10 |
| 53 | A detecting Al ion luminophor 2-(Anthracen-1-yliminomethyl)-phenol: Theoretical investigation on the fluorescence properties and ESIPT mechanism. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 208, 309-314 | 4.4 | 18 |
| 52 | Doping-induced negative differential conductance enhancement in single-molecule junction. *Physica E: Low-Dimensional Systems and Nanostructures*, **2019**, 106, 270-276 | 3 | 12 |
| 51 | A theoretical study on the ESPT mechanism for a novel Bis-HPBT fluorophore. *Journal of Physical Organic Chemistry*, **2018**, 31, e3821 | 2.1 | 7 |
| 50 | Globally Accurate Potential Energy Surface for HCS(AA?) by Extrapolation to the Complete Basis Set Limit. *Journal of Physical Chemistry A*, **2018**, 122, 4390-4398 | 2.8 | 10 |
| 49 | Accurate global potential energy surface for the ground state of CH by extrapolation to the complete basis set limit.. *RSC Advances*, **2018**, 8, 13635-13642 | 3.7 | 10 |

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| 48 | Electrically enhanced hot hole driven oxidation catalysis at the interface of a plasmon-exciton hybrid. *Nanoscale*, **2018**, 10, 5482-5488 | 7.7 | 90 |
| 47 | The manifestation of vibrational excitation effect in reactions C + SH(v= 0□0,j= 0) $ rightarrow $ H + CS, S + CH. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2018**, 51, 065202 | 1.3 | 9 |
| 46 | Theoretical investigation on excited state intramolecular proton transfer of 1-aryl-2-(furan-2-yl) butane-1, 3-diones substitutions. *Journal of Molecular Structure*, **2018**, 1173, 341-344 | 3.4 | 13 |
| 45 | A global potential energy surface for H2S+(X 4A??) and quasi-classical trajectory study of the S+(4S) + H2(X1□g) reaction. *Molecular Physics*, **2018**, 116, 129-141 | 1.7 | 14 |
| 44 | Exciton-plasmon coupling interactions: from principle to applications. *Nanophotonics*, **2018**, 7, 145-167 | 6.3 | 95 |
| 43 | Excited state intramolecular proton transfer mechanism of o-hydroxynaphthyl phenanthroimidazole. *Chinese Physics B*, **2018**, 27, 023103 | 1.2 | 14 |
| 42 | The order of multiple excited state proton transfer in ternary complex of norharmane and acetic acids. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 202, 30-35 | 4.4 | 14 |
| 41 | A theoretical investigation on excited-state single or double proton transfer process for aloesaponarin I. *Canadian Journal of Chemistry*, **2018**, 96, 83-88 | 0.9 | 9 |
| 40 | Novel potential energy surface-based quantum dynamics of ion□olecule reaction ${{rm{O}}}^{+}+{{rm{D}}}_{2}to {mathrm{OD}}^{+}+{rm{D}}$. *Chinese Physics B*, **2018**, 27, 043104 | 1.2 | 5 |
| 39 | Quantum dynamics calculations for O+ + H2 (vi = 0, ji = 0) -> OH+ + H ion□olecule reaction on a new potential energy surface. *European Physical Journal D*, **2018**, 72, 1 | 1.3 | 3 |
| 38 | Accurate potential energy surface of HS( ?) via extrapolation to the complete basis set limit and its use in dynamics study of reaction. *Journal of Chemical Physics*, **2018**, 149, 154303 | 3.9 | 15 |
| 37 | Exciton-plasmon hybrids for surface catalysis detected by SERS. *Nanotechnology*, **2018**, 29, 372001 | 3.4 | 15 |
| 36 | Exploring the reaction dynamics of O(3P)+ (X2 )->OH+(X3□)+ H(2S) reaction with time-dependent wave packet method. *International Journal of Quantum Chemistry*, **2017**, 117, e25343 | 2.1 | 5 |
| 35 | A globally accurate potential energy surface of (mathrm{HS_2}{(A,^2A^prime )}) and studies on the reaction dynamic of (mathrm{H}(^2mathrm{S})+mathrm{S_2}(a,^1{varDelta }_g)). *Theoretical Chemistry Accounts*, **2017**, 136, 1 | 1.9 | 7 |
| 34 | Recent advances in surface plasmon-driven catalytic reactions. *RSC Advances*, **2017**, 7, 31189-31203 | 3.7 | 46 |
| 33 | Effect of HO Adsorption on Negative Differential Conductance Behavior of Single Junction. *Scientific Reports*, **2017**, 7, 4195 | 4.9 | 7 |
| 32 | Electrooptical Synergy on Plasmon□Exciton-Codriven Surface Reduction Reactions. *Advanced Materials Interfaces*, **2017**, 4, 1700869 | 4.6 | 82 |
| 31 | Accurate Theoretical Study of LiS Radical and Its Singly Charged Cation and Anion in their Ground Electronic State. *Chinese Journal of Chemical Physics*, **2017**, 30, 128-134 | 0.9 | 3 |

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| 30 | Solvent Effects on Two-Photon Absorption of Alkyne and Alkene Bridging Chromophores. *Chinese Journal of Chemical Physics*, **2017**, 30, 63-70 | 0.9 | 1 |
| 29 | The stereodynamics study on the isotopic substitution C + SH(D, T) -> H(D, T) + CS reactions on the new HCS(X2A? ) potential energy surface. *Canadian Journal of Physics*, **2017**, 95, 1219-1224 | 1.1 | 7 |
| 28 | Numerical simulation of evolution features of the atmospheric-pressure CF4 plasma generated by the pulsed dielectric barrier discharge. *European Physical Journal D*, **2016**, 70, 1 | 1.3 | 12 |
| 27 | Accurate double many-body expansion potential energy surface of HS 2 A 2 A?) by scaling the external correlation. *Chinese Physics B*, **2016**, 25, 053101 | 1.2 | 5 |
| 26 | Globally accurate potential energy surface for the ground-state HCS(XA?) and its use in reaction dynamics. *Scientific Reports*, **2016**, 6, 37734 | 4.9 | 13 |
| 25 | Particle Densities of the Atmospheric-Pressure Argon Plasmas Generated by the Pulsed Dielectric Barrier Discharges. *Plasma Science and Technology*, **2016**, 18, 1081-1088 | 1.5 | 7 |
| 24 | Coriolis coupling effects in the H+Li2(X1g+)->LiH(X1)+Li reaction: A time-dependent wave packet investigation. *Chemical Physics Letters*, **2016**, 651, 233-237 | 2.5 | 22 |
| 23 | Accurate theoretical study on the ground and first-excited states of Na2: potential energy curves, spectroscopic parameters, and vibrational energy levels. *Canadian Journal of Physics*, **2016**, 94, 1259-1264 | 1.1 | 4 |
| 22 | Effect of thiophene rings on UV/visible spectra and non-linear optical (NLO) properties of triphenylamine based dyes: a quantum chemical perspective. *Journal of Physical Organic Chemistry*, **2015**, 28, 418-422 | 2.1 | 32 |
| 21 | The quantum dynamics of the reactions N+H2(HD,D2) and their vibrational excitation effect. *International Journal of Quantum Chemistry*, **2015**, 115, 231-238 | 2.1 | 6 |
| 20 | Globally accurate ab initio based potential energy surface of H 2 O + ( X 4 A?). *Chinese Physics B*, **2015**, 24, 063101 | 1.2 | 13 |
| 19 | Accurate adiabatic potential energy surface for 12A? state of FH2 based on ab initio data extrapolated to the complete basis set limit. *European Physical Journal D*, **2015**, 69, 1 | 1.3 | 8 |
| 18 | Cross sections for vibrational inhibition at low collision energies for the reaction H + Li2(X1g ) -> Li + LiH (X1). *European Physical Journal D*, **2015**, 69, 1 | 1.3 | 26 |
| 17 | Theoretical Analysis on Optical Limiting Properties of Newly Synthesized Graphene Oxide-Porphyrin Composites. *Chinese Journal of Chemical Physics*, **2015**, 28, 257-262 | 0.9 | 4 |
| 16 | Accurate ab initio -based analytical potential energy function for S 2 ( 1 g ) via extrapolation to the complete basis set limit. *Chinese Physics B*, **2015**, 24, 013101 | 1.2 | 10 |
| 15 | Accurate potential energy curve and spectroscopic properties of S2(b1g+) via extrapolation to the complete basis set limit. *Physica Scripta*, **2015**, 90, 035403 | 2.6 | 8 |
| 14 | The NLO properties of hybrid materials based on molybdate/hexamolybdate derivatives: A theoretical perspective for electro-optic modulation. *Synthetic Metals*, **2014**, 198, 277-284 | 3.6 | 4 |
| 13 | Effect of reagent vibrational excitation on reaction S(3P)+D2 in 3A? and 3A? states. *Computational and Theoretical Chemistry*, **2014**, 1039, 15-20 | 2 | 5 |

# List of Publications

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|---|---|---|---|
| 12 | A typical slow reaction H( 2 S) + S 2 ( X 3 Σg ) -> SH( X 2 Π) + S( 3 P) on a new surface: Quantum dynamics calculations. *Chinese Physics B*, **2014**, 23, 073101 | 1.2 | 8 |
| 11 | Variation of Two-Photon Absorption Cross Sections and Optical Limiting of Compounds Induced by Static Electric Field. *Chinese Journal of Chemical Physics*, **2014**, 27, 259-264 | 0.9 | 2 |
| 10 | Dynamical properties of S(3P) + HD reaction on 13A?state and their quantum wavepacket calculation. *International Journal of Quantum Chemistry*, **2014**, 114, 748-754 | 2.1 | 8 |
| 9 | Accurate ab initio-based DMBE potential energy surface for HLi2(X 2A?) via scaling of the external correlation. *European Physical Journal D*, **2014**, 68, 1 | 1.3 | 13 |
| 8 | Effect of π-conjugation spacer (CC) on the first hyperpolarizabilities of polymeric chain containing polyoxometalate cluster as a side-chain pendant: A DFT study. *Computational and Theoretical Chemistry*, **2012**, 994, 34-40 | 2 | 93 |
| 7 | Ab initio-based double many-body expansion potential energy surface for the first excited triplet state of the ammonia molecule. *Journal of Chemical Physics*, **2012**, 136, 194705 | 3.9 | 25 |
| 6 | Accurate double many-body expansion potential energy surface for ground-state HS2 based on ab initio data extrapolated to the complete basis set limit. *Journal of Physical Chemistry A*, **2011**, 115, 5274-83 | 2.8 | 24 |
| 5 | Potential energy surface for ground-state H2S via scaling of the external correlation, comparison with extrapolation to complete basis set limit, and use in reaction dynamics. *Journal of Physical Chemistry A*, **2009**, 113, 9213-9 | 2.8 | 25 |
| 4 | Accurate ab initio double many-body expansion potential energy surface for ground-state H2S by extrapolation to the complete basis set limit. *Journal of Chemical Physics*, **2009**, 130, 134317 | 3.9 | 47 |
| 3 | A comparison of single-reference coupled-cluster and multi-reference configuration interaction methods for representative cuts of the potential energy surface. *Computational and Theoretical Chemistry*, **2008**, 859, 22-29 | | 14 |
| 2 | Solvent effects on two-photon absorption cross sections of a newly synthesized polymerization initiator. *Computational and Theoretical Chemistry*, **2006**, 772, 75-79 | | 11 |
| 1 | Dynamical behavior of ultra-short laser pulse in a cascade three-level molecular system. *Wuli Xuebao/Acta Physica Sinica*, **2006**, 55, 1803 | 0.6 | 6 |