

# Jia-Dan Xue

## List of Publications by Year in descending order

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63  
papers

809  
citations

516710

16  
h-index

580821

25  
g-index

63  
all docs

63  
docs citations

63  
times ranked

762  
citing authors

#	ARTICLE	IF	CITATIONS
1	A building-block design for enhanced visible-light switching of diarylethenes. <i>Nature Communications</i> , 2019, 10, 4232.	12.8	105
2	Time-Resolved Resonance Raman Identification and Structural Characterization of a Light Absorbing Transient Intermediate in the Photoinduced Reaction of Benzophenone in 2-Propanol. <i>Journal of Organic Chemistry</i> , 2007, 72, 7148-7156.	3.2	41
3	Engineering Fatty Acid Photodecarboxylase to Enable Highly Selective Decarboxylation of <i>trans</i> -Fatty Acids. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20695-20699.	13.8	40
4	Short-time dynamics of 2-thiouracil in the light absorbing S <sub>2</sub> ( $\hat{\epsilon}$ ) state. <i>Journal of Chemical Physics</i> , 2015, 143, 175103.	3.0	27
5	Raman and terahertz spectroscopical investigation of cocrystal formation process of piracetam and 3-hydroxybenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 488-494.	3.9	26
6	Resonance Raman Spectroscopic and Theoretical Investigation of the Excited State Proton Transfer Reaction Dynamics of 2-Thiopyridone. <i>Journal of Physical Chemistry B</i> , 2011, 115, 8266-8277.	2.6	25
7	Pharmaceutical Cocrystal Formation of Pyrazinamide with 3-Hydroxybenzoic Acid: A Terahertz and Raman Vibrational Spectroscopies Study. <i>Molecules</i> , 2019, 24, 488.	3.8	25
8	Photoconversion of $\hat{I}^2$ -Lapachone to $\hat{I}^{\pm}$ -Lapachone via a Protonation-Assisted Singlet Excited State Pathway in Aqueous Solution: A Time-Resolved Spectroscopic Study. <i>Journal of Organic Chemistry</i> , 2015, 80, 7340-7350.	3.2	24
9	Structural investigation of the cocrystal formed between 5-fluorocytosine and fumaric acid based on vibrational spectroscopic technique. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 178, 251-257.	3.9	24
10	Vibrational spectroscopic study of polymorphism and polymorphic transformation of the anti-viral drug lamivudine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 1158-1163.	3.9	22
11	Solid phase drug-drug pharmaceutical co-crystal formed between pyrazinamide and diflunisal: Structural characterization based on terahertz/Raman spectroscopy combining with DFT calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 234, 118265.	3.9	22
12	Investigation into tautomeric polymorphism of 2-thiobarbituric acid using experimental vibrational spectroscopy combined with DFT theoretical simulation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 204, 99-104.	3.9	20
13	Solid-state cocrystal formation between acyclovir and fumaric acid: Terahertz and Raman vibrational spectroscopic studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 186, 29-36.	3.9	19
14	Local order and vibrational coupling of the C=O Stretching Mode of $\hat{I}^3$ -Caprolactone in liquid binary mixtures. <i>Scientific Reports</i> , 2017, 7, 12182.	3.3	18
15	Co-Crystal Formation of Antibiotic Nitrofurantoin Drug and Melamine Co-Former Based on a Vibrational Spectroscopic Study. <i>Pharmaceutics</i> , 2019, 11, 56.	4.5	18
16	Macromolecular Chiral Amplification through a Random Coil to One-Handed Helix Transformation Induced by Metal Ion Coordination in an Aqueous Solution. <i>Macromolecules</i> , 2020, 53, 6002-6017.	4.8	17
17	Vibrational spectral and structural characterization of multicomponent ternary co-crystal formation within acetazolamide, nicotinamide and 2-pyridone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 245, 118885.	3.9	17
18	Investigation of Polymorphism and Cocrystallization of Active Pharmaceutical Ingredients Using Vibrational Spectroscopic Techniques. <i>Current Pharmaceutical Design</i> , 2016, 22, 4917-4928.	1.9	16

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19	Environment-dependent conformation investigation of 3-amino-1,2,4-triazole (3-AT): Raman Spectroscopy and density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 478-485.	3.9	15
20	Investigation into structure and dehydration dynamic of gallic acid monohydrate: A Raman spectroscopic study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 201, 128-133.	3.9	15
21	Terahertz and Raman Spectroscopic Investigation of Monohydrate Cocrystal of Antitubercular Isoniazid with Protocatechuic Acid. <i>Pharmaceutics</i> , 2021, 13, 1303.	4.5	15
22	Time-resolved spectroscopic and density functional theory investigation of the photochemistry of suprofen. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 117-125.	2.5	14
23	Raman and Terahertz Spectroscopic Investigation of Cocrystal Formation Involving Antibiotic Nitrofurantoin Drug and Coformer 4-aminobenzoic Acid. <i>Crystals</i> , 2016, 6, 164.	2.2	13
24	UV and Resonance Raman Spectroscopic and Theoretical Studies on the Solvent-Dependent Ground and Excited-State Thione $\rightleftharpoons$ Thiol Tautomerization of 4,6-Dimethyl-2-mercaptopyrimidine (DMMP). <i>Journal of Physical Chemistry A</i> , 2018, 122, 5710-5720.	2.5	13
25	Structural investigation of a 2:1 co-crystal between diflunisal and isonicotinamide based on terahertz and Raman spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 216, 98-104.	3.9	13
26	Spectroscopic investigation on structure and pH dependent Cocrystal formation between gamma-aminobutyric acid and benzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 377-381.	3.9	11
27	Vibrational Spectroscopic Investigation into Novel Ternary Eutectic Formed between Pyrazinamide, Fumaric Acid, and Isoniazid. <i>ACS Omega</i> , 2020, 5, 17266-17274.	3.5	11
28	Solvent-dependent dynamics of hydrogen bonding structure 5-(methylthio)-1,3,4-thiadiazole-2(3H)-thione as determined by Raman spectroscopy and theoretical calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 470-477.	3.9	10
29	UV-Vis, Fluorescence, and Resonance Raman Spectroscopic and Density Functional Theoretical Studies on 3-Amino-1,2,4-triazole: Microsolvation and Solvent-Dependent Nonadiabatic Excited State Decay in Solution. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8530-8538.	2.5	10
30	Structure and spectroscopic characterization of pharmaceutical co-crystal formation between acetazolamide and 4-hydroxybenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 219, 419-426.	3.9	10
31	Structural dynamics of 4-cyanobenzaldehyde in $S_{2(1)}$ ( $\dot{\nu}^*$ ) state. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 105-113.	2.5	9
32	Structural insights into anhydrous and monohydrated forms of 2,4,6-trihydroxybenzoic acid based on Raman and terahertz spectroscopic characterization. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117436.	3.9	9
33	Decay Dynamics of 3-methylacrylonitrile from the light absorbing $S_{2(1)}$ ( $\dot{\nu}^*$ ) state $\bullet$ . Resonance Raman Spectroscopy and CASSCF Study. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 438-447.	2.5	8
34	Solvent-dependent structural dynamics of 2(1 <i>H</i> )-pyridinone in light absorbing $S_{4(1)}$ ( $\dot{\nu}^*$ ) state. <i>Journal of Raman Spectroscopy</i> , 2016, 47, 299-309.	2.5	8
35	Influence of Water in the Photogeneration and Properties of a Bifunctional Quinone Methide. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11132-11141.	2.6	8
36	Structural investigation of anhydrous nitrofurantoin and its monohydrate based on terahertz/Raman vibrational spectroscopy and density functional theory. <i>Journal of Molecular Structure</i> , 2018, 1153, 170-178.	3.6	7

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37	Hydrogen bond configuration and protonation of ground and lowest excited triplet states of 4-aminobiphenyl based on nanosecond transient absorption spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 217, 44-50.	3.9	7
38	Theoretical studies on the photochemistry of 2-nitrofluorene in the gas phase and acetonitrile solution. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16772-16782.	2.8	7
39	UV-Vis, Raman spectroscopic and density functional theoretical studies on microsolvation of 1,2,4-triazole-3-thione clusters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 258, 119762.	3.9	7
40	Excited State Proton Transfer Dynamics of Thioacetamide in the S <sub>2</sub> (ππ*) State: Resonance Raman Spectroscopic and Quantum Mechanical Calculations Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 832-842.	2.5	6
41	Direct observation of stepwise intermolecular proton and hydrogen transfer between alcohols and the triplet state of 4-nitro-1-naphthol. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11876-11881.	2.8	6
42	Intermolecular Hydrogen Abstraction from Hydroxy Group and Alkyl by T <sub>1</sub> (ππ*) of 1-Chloro-4-nitronaphthalene. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1831-1837.	2.5	5
43	Ab Initio Study of Decay Dynamics of 1-Nitronaphthalene Initiated from the S <sub>2</sub> (ππ*) State. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10784-10791.	2.5	5
44	Solvent effect on the initial structural dynamics of benzaldehyde in the S <sub>3</sub> (ππ*) state: Resonance Raman spectroscopic study. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 684-695.	2.5	5
45	Engineering Fatty Acid Photodecarboxylase to Enable Highly Selective Decarboxylation of trans-Fatty Acids. <i>Angewandte Chemie</i> , 2021, 133, 20863-20867.	2.0	5
46	Direct observation of transient species generated from protonation and deprotonation of the lowest triplet of p-nitrophenylphenol. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 635-641.	1.3	5
47	Structural Dynamics of 3-Dimethylamino-2-methyl-propenal in S <sub>2</sub> (ππ*) State. <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 149-158.	1.3	4
48	Nonadiabatic decay dynamics of phthalide from the light-absorbing S <sub>3</sub> (ππ*) state: resonance Raman spectroscopy and CASSCF study. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 1201-1211.	2.5	4
49	Absorption, fluorescence, Raman spectroscopic and density functional theoretical studies on the singlet and triplet excited state decay of 3-amino-5-mercapto-1,2,4-triazole. <i>RSC Advances</i> , 2020, 10, 13442-13450.	3.6	4
50	Effect of the weak intermolecular C-H...O=C hydrogen bonding, solvent polarity and concentration on the frequency of the C=O stretch mode of 2-thiophenecarboxaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 255, 119651.	3.9	4
51	Raman and Terahertz Spectroscopic Characterization of Solid-state Cocrystal Formation within Specific Active Pharmaceutical Ingredients. <i>Current Pharmaceutical Design</i> , 2020, 26, 4829-4846.	1.9	4
52	Decay dynamics of 1,2-carboxylic methyl esters (CH <sub>3</sub> OCOCH:CHR) in the lower-lying excited states: Resonance Raman and complete active space self-consistent field calculation study. <i>Journal of Chemical Physics</i> , 2014, 141, 134312.	3.0	3
53	Direct Observation of 4-Phenoxyphenylnitrenium Ion: A Transient Absorption and Transient Resonance Raman Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14720-14727.	2.6	3
54	Structural Dynamics of Phenyl Azide in Light-Absorbing Excited States: Resonance Raman and Quantum Mechanical Calculation Study. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 21-30.	1.3	3

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55	Short-time dynamics and decay mechanism of 2(1 <i>H</i> )-pyridinone upon excitation to the light-absorbing S <sub>4</sub> (21??*) state. <i>Journal of Chemical Physics</i> , 2017, 146, 114305.	3.0	3
56	Decay dynamics of 6-azauracil from the light absorbing S <sub>2</sub> (i??*) state. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 345-359.	2.5	3
57	Resonance Raman spectroscopic and density functional theoretical study on microsolvated 2-Thiocyosine clusters with polar solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 230, 118043.	3.9	3
58	Electron transfer from guanosine to the lowest triplet excited state of 4-nitroindole through hydrogen-bonded complex. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 408, 113106.	3.9	3
59	Excited-state proton transfer via higher excited state in 2-mercaptobenzothiazole: Absorption, fluorescence, Raman spectroscopic study, and theoretical calculation. <i>Journal of Raman Spectroscopy</i> , 2020, 51, 125-132.	2.5	2
60	Structural dynamics of phenylisothiocyanate in the light-absorbing excited states: Resonance Raman and complete active space self-consistent field calculation study. <i>Journal of Chemical Physics</i> , 2014, 140, 194305.	3.0	1
61	Decay Dynamics of N, N-Dimethylthioacetamide in S <sub>3</sub> (i??*) State. <i>Chinese Journal of Chemical Physics</i> , 2015, 28, 27-34.	1.3	1
62	Structural dynamics of 4-formaldehyde imidazole and imidazole in light absorbing S <sub>2</sub> (i??*) state. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 293-301.	2.5	1
63	Short-time dynamics and decay mechanism of E,E-2,4-hexadienal in the first light-absorbing S <sub>2</sub> (i??*) state. <i>Journal of Chemical Physics</i> , 2019, 151, 234303.	3.0	0