

# Jia-Dan Xue

## List of Publications by Year in descending order

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63  
papers

809  
citations

516710

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h-index

580821

25  
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63  
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63  
docs citations

63  
times ranked

762  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
3	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
4	Terahertz and Raman Spectroscopic Investigation of Monohydrate Cocrystal of Antitubercular Isoniazid with Protocatechuic Acid. <i>Pharmaceutics</i> , 2021, 13, 1303.	4.5	15
5	Engineering Fatty Acid Photodecarboxylase to Enable Highly Selective Decarboxylation of <i>trans</i> -Fatty Acids. <i>Angewandte Chemie</i> , 2021, 133, 20863-20867.	2.0	5
6	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
7	UV-Vis, Raman spectroscopic and density functional theoretical studies on microsolvation 1, 2, 4-triazole-3-thione clusters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 258, 119762.	3.9	7
8	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
9	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
10	Resonance Raman spectroscopic and density functional theoretical study on microsolvated 2-Thiocytosine clusters with polar solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 230, 118043.	3.9	3
11	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
12	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
13	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
14	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
15	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
16	Direct observation of transient species generated from protonation and deprotonation of the lowest triplet of <i>p</i> -nitrophenylphenol. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 635-641.	1.3	5
17	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
18	A building-block design for enhanced visible-light switching of diarylethenes. <i>Nature Communications</i> , 2019, 10, 4232.	12.8	105

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19	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
20	Decay dynamics of 6-azauracil from the light absorbing S <sub>2</sub> (ĪĪ*) state. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 345-359.	2.5	3
21	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
22	Hydrogen bond configuration and protonation of ground and lowest excited triplet states of 4-aminobenzonitrophenyl based on nanosecond transient absorption spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 217, 44-50.	3.9	7
23	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
24	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
25	Solvent effect on the initial structural dynamics of benzaldehyde in the S <sub>3</sub> (ĪĪ*) state—Resonance Raman spectroscopic study. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 684-695.	2.5	5
26	Short-time dynamics and decay mechanism of E,E-2,4-hexadienal in the first light-absorbing S <sub>2</sub> (ĪĪ*) state. <i>Journal of Chemical Physics</i> , 2019, 151, 234303.	3.0	0
27	Intermolecular Hydrogen Abstraction from Hydroxy Group and Alkyl by T <sub>1</sub> (ĪĪ*) of 1-Chloro-4-nitronaphthalene. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1831-1837.	2.5	5
28	Ab Initio Study of Decay Dynamics of 1-Nitronaphthalene Initiated from the S <sub>2</sub> (ĪĪ*) T <sub>1</sub> ETQ <sub>0,0</sub> rgBT <sub>5</sub> /Overlock	2.5	5
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	UV and Resonance Raman Spectroscopic and Theoretical Studies on the Solvent-Dependent Ground and Excited-State Thione ↔ Thiol Tautomerization of 4,6-Dimethyl-2-mercaptopyrimidine (DMMP). <i>Journal of Physical Chemistry A</i> , 2018, 122, 5710-5720.	2.5	13

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37	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
38	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
39	Short-time dynamics and decay mechanism of 2(1 <i>H</i> )-pyridinone upon excitation to the light-absorbing S <sub>4</sub> ( $\pi\pi^*$ ) state. <i>Journal of Chemical Physics</i> , 2017, 146, 114305.	3.0	3
40	Nonadiabatic decay dynamics of phthalide from the light-absorbing S <sub>3</sub> ( $\pi\pi^*$ ) state—resonance Raman spectroscopy and CASSCF study. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 1201-1211.	2.5	4
41	Local order and vibrational coupling of the C=O Stretching Mode of $\hat{\beta}$ -Caprolactone in liquid binary mixtures. <i>Scientific Reports</i> , 2017, 7, 12182.	3.3	18
42	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
43	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
44	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
45	Solvent-dependent structural dynamics of 2(1 <i>H</i> )-pyridinone in light absorbing S <sub>4</sub> ( $\pi\pi^*$ ) state. <i>Journal of Raman Spectroscopy</i> , 2016, 47, 299-309.	2.5	8
46	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
47	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
48	Short-time dynamics of 2-thiouracil in the light absorbing S <sub>2</sub> ( $\pi\pi^*$ ) state. <i>Journal of Chemical Physics</i> , 2015, 143, 175103.	3.0	27
49	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
50	Decay Dynamics of N, N-Dimethylthioacetamide in S <sub>3</sub> ( $\pi\pi^*$ ) State. <i>Chinese Journal of Chemical Physics</i> , 2015, 28, 27-34.	1.3	1
51	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
52	Structural dynamics of 4-formaldehyde imidazole and imidazole in light absorbing S <sub>2</sub> ( $\pi\pi^*$ ) state. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 293-301.	2.5	1
53	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
54	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

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55	Excited State Proton Transfer Dynamics of Thioacetamide in $S_{2/2}$ ( $\tilde{\pi}\pi^*$ ) State: Resonance Raman Spectroscopic and Quantum Mechanical Calculations Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 832-842.	2.5	6
56	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
57	Structural Dynamics of 3-Dimethylamino-2-methyl-propenal in $S_2(\tilde{\pi}\pi^*)$ State. <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 149-158.	1.3	4
58	Decay Dynamics of 3-methylacrylonitrile from the light absorbing $S_{2/2}$ ( $\tilde{\pi}\pi^*$ ) state â€• Resonance Raman Spectroscopy and CASSCF Study. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 438-447.	2.5	8
59	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
60	Decay dynamics of $\hat{I}^{\pm}, \hat{I}^2$ -carboxylic methyl esters ( $CH_3OCOCH:CHR$ ) in the lower-lying excited statesâ€• Resonance Raman and complete active space self-consistent field calculation study. <i>Journal of Chemical Physics</i> , 2014, 141, 134312.	3.0	3
61	Structural dynamics of 4-cyanobenzaldehyde in $S_{2/2}$ ( $\tilde{\pi}\pi^*$ ) state. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 105-113.	2.5	9
62	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
63	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