

Munira Khalil

List of Publications by Year in descending order

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54
papers

1,918
citations

236925

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docs citations

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Femtosecond X-ray Spectroscopy Directly Quantifies Transient Excited-State Mixed Valency. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 378-386.	4.6	9
2	Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer. <i>Nature Chemistry</i> , 2021, 13, 343-349.	13.6	59
3	Resonant Inelastic X-ray Scattering Calculations of Transition Metal Complexes Within a Simplified Time-Dependent Density Functional Theory Framework. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3031-3038.	5.3	16
4	Multimode two-dimensional vibronic spectroscopy. I. Orientational response and polarization-selectivity. <i>Journal of Chemical Physics</i> , 2021, 154, 184201.	3.0	10
5	Multimode two-dimensional vibronic spectroscopy. II. Simulating and extracting vibronic coupling parameters from polarization-selective spectra. <i>Journal of Chemical Physics</i> , 2021, 154, 184202.	3.0	8
6	Ultrafast x-ray pump x-ray probe transient absorption spectroscopy: A computational study and proposed experiment probing core-valence electronic correlations in solvated complexes. <i>Journal of Chemical Physics</i> , 2021, 154, 214107.	3.0	5
7	Revealing the bonding of solvated Ru complexes with valence-to-core resonant inelastic X-ray scattering. <i>Chemical Science</i> , 2021, 12, 3713-3725.	7.4	17
8	Manipulating valence and core electronic excitations of a transition-metal complex using UV/Vis and X-ray cavities. <i>Chemical Science</i> , 2021, 12, 8088-8095.	7.4	9
9	Spectral Signatures of Ultrafast Excited-State Intramolecular Proton Transfer from Computational Multi-edge Transient X-ray Absorption Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9840-9847.	4.6	11
10	Determining the Orientation and Vibronic Couplings between Electronic and Vibrational Coordinates with Polarization-Selective Two-Dimensional Vibrational-Electronic Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1558-1563.	4.6	17
11	Ultrafast spectroscopy and diffraction from XUV to x-ray. <i>Journal of Chemical Physics</i> , 2020, 153, 100401.	3.0	6
12	Implementation of Broadband near-UV Pump Pulses for Ultrafast 2D Electronic-Vibrational Spectroscopy. , 2020, , .		0
13	Ultrafast Charge Transfer and Electron Delocalization in a Cyanide-Bridged Ru-Ru Dimer Investigated with Femtosecond Transient X-Ray and IR Spectroscopies. , 2020, , .		0
14	A Theoretical Study of Polarization Selective Two-Dimensional Vibronic Spectroscopies of Multimode Systems. , 2020, , .		0
15	Vibronic Coherence Evolution in Ultrafast Charge Transfer. , 2020, , .		0
16	Ultrafast Vibronic Phenomena Directly Revealed by Multidimensional Electronic-Vibrational Spectroscopy. , 2020, , .		0
17	Double core hole valence-to-core x-ray emission spectroscopy: A theoretical exploration using time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 144114.	3.0	11
18	Sticky ends in a self-assembling ABA triblock copolymer: the role of ureas in stimuli-responsive hydrogels. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 91-102.	3.4	7

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19	Carboxylate Anchors Act as Exciton Reporters in 1.3 nm Indium Phosphide Nanoclusters. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1833-1839.	4.6	23
20	Vibronic coherence evolution in multidimensional ultrafast photochemical processes. <i>Nature Communications</i> , 2019, 10, 5621.	12.8	38
21	Probing ultrafast vibrational dynamics of intramolecular hydrogen bonds with broadband infrared pump-probe spectroscopy. <i>Chemical Physics</i> , 2019, 519, 38-44.	1.9	13
22	Comprehensive Experimental and Computational Spectroscopic Study of Hexacyanoferrate Complexes in Water: From Infrared to X-ray Wavelengths. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5075-5086.	2.6	40
23	Implementation of continuous fast scanning detection in femtosecond Fourier-transform two-dimensional vibrational-electronic spectroscopy to decrease data acquisition time. <i>Review of Scientific Instruments</i> , 2018, 89, 113104.	1.3	9
24	Mapping Vibronic Couplings in a Solar Cell Dye with Polarization-Selective Two-Dimensional Electronic-Vibrational Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6289-6295.	4.6	31
25	Ultrafast Independent N-H and N-C Bond Deformation Investigated with Resonant Inelastic X-ray Scattering. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6088-6092.	13.8	36
26	Picosecond sulfur K-edge X-ray absorption spectroscopy with applications to excited state proton transfer. <i>Structural Dynamics</i> , 2017, 4, 044021.	2.3	15
27	Signatures of vibronic coupling in two-dimensional electronic-vibrational and vibrational-electronic spectroscopies. <i>Journal of Chemical Physics</i> , 2017, 147, 094202.	3.0	40
28	Untersuchung unabhängiger N-H- und N-C-Bindungsverformungen auf ultrakurzen Zeitskalen mit resonanter inelastischer Ramanstreuung. <i>Angewandte Chemie</i> , 2017, 129, 6184-6188.	2.0	3
29	Innenrücktitelbild: Untersuchung unabhängiger N-H- und N-C-Bindungsverformungen auf ultrakurzen Zeitskalen mit resonanter inelastischer Ramanstreuung (<i>Angew. Chem.</i> 22/2017). <i>Angewandte Chemie</i> , 2017, 129, 6441-6441.	2.0	0
30	Investigating vibrational relaxation in cyanide-bridged transition metal mixed-valence complexes using two-dimensional infrared and infrared pump-probe spectroscopies. <i>Structural Dynamics</i> , 2016, 3, 023609.	2.3	11
31	Compression of tunable broadband mid-IR pulses with a deformable mirror pulse shaper. <i>Journal of the Optical Society of America B: Optical Physics</i> , 2016, 33, 2033.	2.1	8
32	Fourier transform two-dimensional electronic-vibrational spectroscopy using an octave-spanning mid-IR probe. <i>Optics Letters</i> , 2016, 41, 2895.	3.3	41
33	Time-Resolved X-ray Spectroscopy in the Water Window: Elucidating Transient Valence Charge Distributions in an Aqueous Fe(II) Complex. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 465-470.	4.6	50
34	Two-dimensional vibrational-electronic spectroscopy. <i>Journal of Chemical Physics</i> , 2015, 143, 154201.	3.0	58
35	Measuring Coherently Coupled Intramolecular Vibrational and Charge-Transfer Dynamics with Two-Dimensional Vibrational-Electronic Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1286-1292.	4.6	52
36	Simulating Valence-to-Core X-ray Emission Spectroscopy of Transition Metal Complexes with Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5804-5809.	5.3	49

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37	Investigating vibrational anharmonic couplings in cyanide-bridged transition metal mixed valence complexes using two-dimensional infrared spectroscopy. <i>Journal of Chemical Physics</i> , 2014, 140, 084505.	3.0	20
38	pH-Dependent Picosecond Structural Dynamics in the Distal Pocket of Nitrophorin 4 Investigated by 2D IR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15804-15811.	2.6	21
39	Simulating Ru L ₃ -Edge X-ray Absorption Spectroscopy with Time-Dependent Density Functional Theory: Model Complexes and Electron Localization in Mixed-Valence Metal Dimers. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4444-4454.	2.5	59
40	Effect of Solvent Polarity on the Vibrational Dephasing Dynamics of the Nitrosyl Stretch in an Fe ^{II} Complex Revealed by 2D IR Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6234-6243.	2.5	43
41	Generation of tunable octave-spanning mid-infrared pulses by filamentation in gas media. <i>Optics Letters</i> , 2012, 37, 1787.	3.3	33
42	Communication: Probing non-equilibrium vibrational relaxation pathways of highly excited C ₆₀ N stretching modes following ultrafast back-electron transfer. <i>Journal of Chemical Physics</i> , 2012, 136, 241101.	3.0	25
43	Coherent Fifth-Order Visible-Infrared Spectroscopies: Ultrafast Nonequilibrium Vibrational Dynamics in Solution. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7023-7032.	2.5	22
44	Probing the Electronic Structure of a Photoexcited Solar Cell Dye with Transient X-ray Absorption Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1695-1700.	4.6	63
45	Probing the Photoinduced Metal-Nitrosyl Linkage Isomerism of Sodium Nitroprusside in Solution Using Transient Infrared Spectroscopy. <i>Journal of the American Chemical Society</i> , 2011, 133, 5255-5262.	13.7	57
46	Simulating Picosecond Iron K-Edge X-ray Absorption Spectra by ab Initio Methods To Study Photoinduced Changes in the Electronic Structure of Fe(II) Spin Crossover Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10749-10761.	2.5	27
47	On the Role of High-Frequency Intramolecular Vibrations in Ultrafast Back-Electron Transfer Reactions. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2252-2257.	4.6	25
48	Quantum State-Resolved Probing of Strong-Field-Ionized Xenon Atoms Using Femtosecond High-Order Harmonic Transient Absorption Spectroscopy. <i>Physical Review Letters</i> , 2007, 98, 143601.	7.8	107
49	Picosecond X-ray Absorption Spectroscopy of a Photoinduced Iron(II) Spin Crossover Reaction in Solution. <i>Journal of Physical Chemistry A</i> , 2006, 110, 38-44.	2.5	171
50	From The Cover: Conformational changes during the nanosecond-to-millisecond unfolding of ubiquitin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 612-617.	7.1	150
51	Nonlinear Infrared Spectroscopy of Protein Conformational Change during Thermal Unfolding. <i>Journal of Physical Chemistry B</i> , 2004, 108, 15332-15342.	2.6	83
52	Two-Dimensional Infrared Spectroscopy of Antiparallel β -Sheet Secondary Structure. <i>Journal of the American Chemical Society</i> , 2004, 126, 7981-7990.	13.7	267
53	Molecular Structure and Conformational Composition of 3,4-Epoxy-1-butene As Determined by ab Initio Molecular Orbital Calculations, Microwave Spectroscopy, and Gas-Phase Electron Diffraction. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5585-5589.	2.5	3
54	Phase and amplitude control in the formation and detection of rotational wave packets in the E _g ⁺ state of Li ₂ . <i>Journal of Chemical Physics</i> , 1998, 108, 9259-9274.	3.0	39