Munira Khalil

List of Publications by Year
in descending order

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54 papers	1,918 citations	236925 25 h-index	243625 44 g-index
58 all docs	58 docs citations	58 times ranked	2030 citing authors

#	Article	IF	Citations
1	Two-Dimensional Infrared Spectroscopy of Antiparallel Î²-Sheet Secondary Structure. Journal of the American Chemical Society, 2004, 126, 7981-7990.	13.7	267
2	Picosecond X-ray Absorption Spectroscopy of a Photoinduced Iron(II) Spin Crossover Reaction in Solution. Journal of Physical Chemistry A, 2006, 110, 38-44.	2.5	171
3	From The Cover: Conformational changes during the nanosecond-to-millisecond unfolding of ubiquitin. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 612-617.	7.1	150
4	Quantum State-Resolved Probing of Strong-Field-Ionized Xenon Atoms Using Femtosecond High-Order Harmonic Transient Absorption Spectroscopy. Physical Review Letters, 2007, 98, 143601.	7.8	107
5	Nonlinear Infrared Spectroscopy of Protein Conformational Change during Thermal Unfolding. Journal of Physical Chemistry B, 2004, 108, 15332-15342.	2.6	83
6	Probing the Electronic Structure of a Photoexcited Solar Cell Dye with Transient X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2012, 3, 1695-1700.	4.6	63
7	Simulating Ru L₃-Edge X-ray Absorption Spectroscopy with Time-Dependent Density Functional Theory: Model Complexes and Electron Localization in Mixed-Valence Metal Dimers. Journal of Physical Chemistry A, 2013, 117, 4444-4454.	2.5	59
8	Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer. Nature Chemistry, 2021, 13, 343-349.	13.6	59
9	Two-dimensional vibrational-electronic spectroscopy. Journal of Chemical Physics, 2015, 143, 154201.	3.0	58
10	Probing the Photoinduced Metalâ^'Nitrosyl Linkage Isomerism of Sodium Nitroprusside in Solution Using Transient Infrared Spectroscopy. Journal of the American Chemical Society, 2011, 133, 5255-5262.	13.7	57
11	Measuring Coherently Coupled Intramolecular Vibrational and Charge-Transfer Dynamics with Two-Dimensional Vibrationalâ€"Electronic Spectroscopy. Journal of Physical Chemistry Letters, 2015, 6, 1286-1292.	4.6	52
12	Time-Resolved X-ray Spectroscopy in the Water Window: Elucidating Transient Valence Charge Distributions in an Aqueous Fe(II) Complex. Journal of Physical Chemistry Letters, 2016, 7, 465-470.	4.6	50
13	Simulating Valence-to-Core X-ray Emission Spectroscopy of Transition Metal Complexes with Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 5804-5809.	5.3	49
14	Effect of Solvent Polarity on the Vibrational Dephasing Dynamics of the Nitrosyl Stretch in an Fe^{II} Complex Revealed by 2D IR Spectroscopy. Journal of Physical Chemistry A, 2013, 117, 6234-6243.	2.5	43
15	Fourier transform two-dimensional electronic-vibrational spectroscopy using an octave-spanning mid-IR probe. Optics Letters, 2016, 41, 2895.	3.3	41
16	Signatures of vibronic coupling in two-dimensional electronic-vibrational and vibrational-electronic spectroscopies. Journal of Chemical Physics, 2017, 147, 094202.	3.0	40
17	Comprehensive Experimental and Computational Spectroscopic Study of Hexacyanoferrate Complexes in Water: From Infrared to X-ray Wavelengths. Journal of Physical Chemistry B, 2018, 122, 5075-5086.	2.6	40
18	Phase and amplitude control in the formation and detection of rotational wave packets in the Eâ€‰1Î£g+ state of Li2. Journal of Chemical Physics, 1998, 108, 9259-9274.	3.0	39

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19	Vibronic coherence evolution in multidimensional ultrafast photochemical processes. Nature Communications, 2019, 10, 5621.	12.8	38
20	Ultrafast Independent Nâ˜H and Nâ˜C Bond Deformation Investigated with Resonant Inelastic Xâ€Ray Scattering. Angewandte Chemie - International Edition, 2017, 56, 6088-6092.	13.8	36
21	Generation of tunable octave-spanning mid-infrared pulses by filamentation in gas media. Optics Letters, 2012, 37, 1787.	3.3	33
22	Mapping Vibronic Couplings in a Solar Cell Dye with Polarization-Selective Two-Dimensional Electronicâ€“Vibrational Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 6289-6295.	4.6	31
23	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. Journal of Physical Chemistry A, 2011, 115, 10749-10761.	2.5	27
24	On the Role of High-Frequency Intramolecular Vibrations in Ultrafast Back-Electron Transfer Reactions. Journal of Physical Chemistry Letters, 2011, 2, 2252-2257.	4.6	25
25	Communication: Probing non-equilibrium vibrational relaxation pathways of highly excited Câ‰¡N stretching modes following ultrafast back-electron transfer. Journal of Chemical Physics, 2012, 136, 241101.	3.0	25
26	Carboxylate Anchors Act as Exciton Reporters in 1.3 nm Indium Phosphide Nanoclusters. Journal of Physical Chemistry Letters, 2019, 10, 1833-1839.	4.6	23
27	Coherent Fifth-Order Visibleâ€“Infrared Spectroscopies: Ultrafast Nonequilibrium Vibrational Dynamics in Solution. Journal of Physical Chemistry A, 2012, 116, 7023-7032.	2.5	22
28	pH-Dependent Picosecond Structural Dynamics in the Distal Pocket of Nitrophorin 4 Investigated by 2D IR Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 15804-15811.	2.6	21
29	Investigating vibrational anharmonic couplings in cyanide-bridged transition metal mixed valence complexes using two-dimensional infrared spectroscopy. Journal of Chemical Physics, 2014, 140, 084505.	3.0	20
30	Determining the Orientation and Vibronic Couplings between Electronic and Vibrational Coordinates with Polarization-Selective Two-Dimensional Vibrational-Electronic Spectroscopy. Journal of Physical Chemistry Letters, 2020, 11, 1558-1563.	4.6	17
31	Revealing the bonding of solvated Ru complexes with valence-to-core resonant inelastic X-ray scattering. Chemical Science, 2021, 12, 3713-3725.	7.4	17
32	Resonant Inelastic X-ray Scattering Calculations of Transition Metal Complexes Within a Simplified Time-Dependent Density Functional Theory Framework. Journal of Chemical Theory and Computation, 2021, 17, 3031-3038.	5.3	16
33	Picosecond sulfur K-edge X-ray absorption spectroscopy with applications to excited state proton transfer. Structural Dynamics, 2017, 4, 044021.	2.3	15
34	Probing ultrafast vibrational dynamics of intramolecular hydrogen bonds with broadband infrared pump-probe spectroscopy. Chemical Physics, 2019, 519, 38-44.	1.9	13
35	Investigating vibrational relaxation in cyanide-bridged transition metal mixed-valence complexes using two-dimensional infrared and infrared pump-probe spectroscopies. Structural Dynamics, 2016, 3, 023609.	2.3	11
36	Double core hole valence-to-core x-ray emission spectroscopy: A theoretical exploration using time-dependent density functional theory. Journal of Chemical Physics, 2019, 151, 144114.	3.0	11

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37	Spectral Signatures of Ultrafast Excited-State Intramolecular Proton Transfer from Computational Multi-edge Transient X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2021, 12, 9840-9847.	4.6	11
38	Multimode two-dimensional vibronic spectroscopy. I. Orientational response and polarization-selectivity. Journal of Chemical Physics, 2021, 154, 184201.	3.0	10
39	Implementation of continuous fast scanning detection in femtosecond Fourier-transform two-dimensional vibrational-electronic spectroscopy to decrease data acquisition time. Review of Scientific Instruments, 2018, 89, 113104.	1.3	9
40	Manipulating valence and core electronic excitations of a transition-metal complex using UV/Vis and X-ray cavities. Chemical Science, 2021, 12, 8088-8095.	7.4	9
41	Femtosecond X-ray Spectroscopy Directly Quantifies Transient Excited-State Mixed Valency. Journal of Physical Chemistry Letters, 2022, 13, 378-386.	4.6	9
42	Compression of tunable broadband mid-IR pulses with a deformable mirror pulse shaper. Journal of the Optical Society of America B: Optical Physics, 2016, 33, 2033.	2.1	8
43	Multimode two-dimensional vibronic spectroscopy. II. Simulating and extracting vibronic coupling parameters from polarization-selective spectra. Journal of Chemical Physics, 2021, 154, 184202.	3.0	8
44	Sticky ends in a self-assembling ABA triblock copolymer: the role of ureas in stimuli-responsive hydrogels. Molecular Systems Design and Engineering, 2019, 4, 91-102.	3.4	7
45	Ultrafast spectroscopy and diffraction from XUV to x-ray. Journal of Chemical Physics, 2020, 153, 100401.	3.0	6
46	Ultrafast x-ray pump x-ray probe transient absorption spectroscopy: A computational study and proposed experiment probing core-valence electronic correlations in solvated complexes. Journal of Chemical Physics, 2021, 154, 214107.	3.0	5
47	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. Journal of Physical Chemistry A, 1999, 103, 5585-5589.	2.5	3
48	Untersuchung unabhÃngiger Nâ€Hâ€•und Nâ€Câ€Bindungsverformungen auf ultrakurzen Zeitskalen mit resonanter inelastischer RÃ¶ntgenstreuung. Angewandte Chemie, 2017, 129, 6184-6188.	2.0	3
49	InnenrÃ¼cktitelbild: Untersuchung unabhÃngiger Nâ€Hâ€•und Nâ€Câ€Bindungsverformungen auf ultrakurzen Zeitskalen mit resonanter inelastischer RÃ¶ntgenstreuung (Angew. Chem. 22/2017). Angewandte Chemie, 2017, 129, 6441-6441.	2.0	0
50	Implementation of Broadband near-UV Pump Pulses for Ultrafast 2D Electronic-Vibrational Spectroscopy. , 2020, , .		0
51	Ultrafast Charge Transfer and Electron Delocalization in a Cyanide-Bridged Ru-Ru Dimer Investigated with Femtosecond Transient X-Ray and IR Spectroscopies. , 2020, , .		0
52	A Theoretical Study of Polarization Selective Two-Dimensional Vibronic Spectroscopies of Multimode Systems. , 2020, , .		0
53	Vibronic Coherence Evolution in Ultrafast Charge Transfer. , 2020, , .		0
54	Ultrafast Vibronic Phenomena Directly Revealed by Multidimensional Electronic-Vibrational Spectroscopy. , 2020, , .		0