Kelly J. Gaffney

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Education

2001 Ph.D. Chemistry University of California, Berkeley, CA
 1993 B.S. Chemistry The Evergreen State College, Olympia, WA

Professional Experience

Interim Associate Laboratory Director Energy Sciences Directorate, 2023-present Chemical Sciences Division Director Energy Sciences Directorate, 2019-2023 Deputy Associate Laboratory Director Energy Sciences Directorate, 2019-2023

Associate Laboratory Director Stanford Synchrotron Radiation Lightsource, 2014-2019

Professor Photon Science, SLAC, Stanford University, 2023-present
Associate Professor Photon Science, SLAC, Stanford University, 2013-2023
Assistant Professor Photon Science, SLAC, Stanford University, 2004-2013
Postdoctoral Research Associate Stanford Synchrotron Radiation Lightsource, 2003-2004

Postdoctoral Research Associate Stanford University, 2001-2003

Analytical Chemist BOC Gases, 1993-1995

Research Interests

My research group makes stroboscopic movies of condensed phase chemical transformations with atomic specificity and resolution. We use femtosecond optical and x-ray lasers to measure the ultrafast dynamics of electronic and vibrational degrees of freedom in a wide range of systems. Our current research emphasizes the study of electronic excited state dynamics in transition metal complexes, what dictates the properties of these electronic excited states, and how they can be harnessed for photocatalysis. In these studies we utilize steady state and time resolved optical and x-ray spectroscopy, as well as x-ray scattering.

Leadership

- Participant, Department of Energy Office of Science, Basic Research Needs in Laser Technology Workshop, 2023
- Chair, Photon Science Department SLAC, Stanford University 2020-2023
- Member, Advanced Photon Source Scientific Advisory Committee, 2020-2022
- Participant, Committee of Visitors, Department of Energy Basic Energy Sciences Chemical Sciences, Geosciences and Biosciences Division, 2020
- Council member on the Department of Energy Basic Energy Sciences Council for Chemical Sciences, Geosciences and Biosciences, 2018-present
- Participant, Department of Energy Basic Energy Sciences Roundtable on Opportunities for Basic Research at the Frontiers of XFEL Ultrafast Science, 2017
- Participant, Committee of Visitors, Department of Energy Basic Energy Sciences Chemical Sciences, Geosciences and Biosciences Division, 2017
- Deputy chair, Photon Science department, SLAC, Stanford University, 2013-2014
- Established chemical dynamics research at the SLAC National Accelerator Laboratory facilitated by a grant from the W.M. Keck foundation.
- Led the LCLS ultrafast dynamics x-ray pump-probe (XPP) end-station design group.

Invited Talks

1. Solvation Dynamics at Interfaces and in Hydrogen Bonded Liquids

Lawrence Livermore National Lab Chemical and Materials Science Division

2.	Dynamics of Photoinjected Electrons at Model Molecular Electronic Interfaces		
3.	Hewlett-Packard Lab Quantum Science Research Division Time Resolving the Motions of Molecules at Surfaces and in Liquids	May 9 th	2003
	SLAC Stanford Synchrotron Radiation Lab	Jun 5 th	2003
4.	Imaging Chemical Dynamics with Ultrafast X-rays Stanford Linear Accelerator Center SSRL 31st User's Meeting	Oct 21st	2004
5.	Ultrafast X-ray Studies of Structural Dynamics American Crystallography Association National Meeting	Jun 24 th	2005
6.	Ultrafast X-ray Studies of Structural Dynamic at SLAC SPIE Conference Optics and Photonics National Meeting	Aug 3 rd	2005
7.	Femtosecond X-ray Measurements of Structural Dynamics Gordon Research Conference X-ray Physics	Aug 9 th	2005
8.	Ultrafast X-ray Measurements of Structural Dynamics: technical challenges at the		
0	XX Congress of the International Union of Crystallography	Aug 24 th	2005
9.	Femtosecond X-ray Measurements of Structural Dynamics at the SPPS ALS Users Meeting	Oct 22 nd	2005
10	Femtosecond X-ray Diffraction Studies of Laser Driven Melting at SLAC	OCI 22	2003
	SPIE Conference High Power Laser Ablation 2006 Free electron laser studies of structural dynamics	May 9 th	2006
11.	Ultrafast Dynamics on Surfaces and in Liquids Workshop at SSRL	Oct 11 th	2006
12	Ultrafast Diffuse Scattering Studies of Melting	Oct 11	2000
12.	SSRL User's Meeting	Oct 13th	2006
13.	Making Molecular Movies: ten trillion frames per second		
	SLAC Public Lecture	Dec 12th	2006
14.	Pump Probe Chemical Dynamics		
	Ultrafast X-ray Summer School at SLAC	Jun 20 th	2007
	Research Opportunities at the X-ray Pump Probe Endstation at the LCLS SSRL User's Meeting	Oct 2 nd	2007
16.	Ultrafast x-ray scattering studies of structural dynamics	4	
	American Chemical Society National Meeting	Apr 7 th	2008
	Experimental and theoretical studies of carrier dependent lattice stability in semicon SPIE Conference High Power Laser Ablation 2008	Apr 21 th	2008
18.	Making Molecular Movies	I1 2rd	2000
10	Low Energy Electrodynamics in Solids 2008 X-ray Free Electron Laser Science	Jul 3 rd	2008
19.	Stanford-Berkeley Synchrotron Summer School	Aug 21 th	2008
20	Dynamics of Hydrogen Bond Exchange in Aqueous Electrolyte Solution	Aug 21	2008
20.	DOE Condensed Phase and Interfacial Molecular Science Meeting	Oct 21th	2008
21.	Dynamics of Hydrogen Bond Exchange in Aqueous Electrolyte Solution	00121	2000
	Argonne National Laboratory Chemistry Division Colloquium	Nov 11th	2008
22.	Science Opportunities and Challenges at the X-ray Pump-Probe Endstation at the	LCLS	
	JSSRR National Meeting University of Tokyo	Jan 11 th	2009
23.	Science Opportunities and Challenges at the X-ray Pump-Probe Endstation at the		
	XFEL Colloquium at SPring-8	Jan 13 th	2009
24.	Dynamics of Hydrogen Bond Exchange in Aqueous Electrolyte Solution	T Ooth	2000
25	Western Spectroscopy Association Meeting	Jan 29 th	2009
23.	Ionizing Radiation Induced Chemical Dynamics Studied with Ultrafast X-ray Lase Radiation Chemistry in the 21 st Century	rs Jul 13 th	2009
26	Ionizing Radiation Induced Chemical Dynamics Studied with Ultrafast X-ray Lase		2009
20.	6 th International Workshop on X-ray Radiation Damage	Mar 12 th	2010
27.	Non-equilibrium dynamics studied with femtosecond resolution X-ray scattering		_010
	PHONONS 2010 National Taiwan University	Apr 22 nd	2010
28.	Complex Molecules in Condensed Phases Gordon Research Conference Atomic and Molecular Interactions	Jul 22 nd	2010
20	H-bond Switching and Ligand Exchange Dynamics in Aqueous Ionic Solution	Jui 44	2010
۷۶.	CECAM Vibrational Spectroscopy of Complex Systems	May 23rd	2011
30.	H-bond Switching and Ligand Exchange Dynamics in Aqueous Ionic Solution		_011
	Time Resolved Vibrational Spectroscopy XV	Jun 23rd	2011
31.	How Does Water Solvate Ions?		

	Gordon Research Conference Atomic Physics	Jun 28th	2011
32.	Caught in the Act: X-ray spectroscopy studies of reaction mechanisms ALS Users Meeting	Oct 5 th	2011
33.	Caught in the Act: X-ray spectroscopy studies of reaction mechanisms SSRL/LCLS Users Meeting	Oct 22 nd	2011
34	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I		
	University of Southern California Department of Chemistry Colloquium	Nov 7 th	2011
35.	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I University of California at Irvine Department of Chemistry Colloquium	onic Soluti Nov 8 th	ion 2011
36	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I	_	
50.	University of Pennsylvania Department of Chemistry Colloquium	Jan 19 th	2012
27	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I	-	
31.	Colorado State University Department of Chemistry Colloquium	Feb 2 nd	2012
20			
38.	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I		
20	University of Colorado Department of Chemistry Colloquium	Feb 3 rd	2012
39.	Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynan		2012
4.0	Banff Meeting on Structural Dynamics	Feb 21st	2012
40.	Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynan		
	American Physical Society March Meeting	Feb 27 th	2012
41.	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I		
	MIT Department of Chemistry Colloquium	Apr 10 th	2012
42.	Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynan	nics	
	Argonne Chemical Sciences Colloquium	Apr 16 th	2012
43.	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I	onic Soluti	ion
	University of Chicago Department of Chemistry Colloquium	Apr 17 th	2012
44.	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I	onic Soluti	ion
	University of Illinois at Champaign-Urbana Department of Chemistry Colloquium	Apr 18th	2012
45.	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I		
	University of Wisconsin at Madison Department of Chemistry Colloquium	Apr 20 th	2012
46	Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynan		2012
чо.	Helmholtz Center Berlin Colloquium	May 8 th	2012
17	Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynan	•	2012
4/.	Center for Free Electron Lasers	May 9 th	2012
10		May 9	2012
40.	Vibrational Anisotropy Studies of Chemical Dynamics Max Born Institute Berlin	May 11 th	2012
40		•	
49.	Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous I		
5 0	University of California at San Diego Department of Chemistry Colloquium	May 22 nd	2012
50.	Ion Recognition and Assembly: Mechanistic studies of ligand exchange in aqueous		2012
~ 1	Telluride Science Research Center	Jul 3 rd	2012
51.	Tracking Non-Adiabatic Electron Transfer Dynamics with X-ray Spectroscopy	. oth	2012
	Gordon Research Conference Electron Donor-Acceptor Interactions	Aug 8th	2012
52.	Ultrafast X-ray Laser Studies of Coupled Electronic and Nuclear Dynamics		• • • •
	Ginzton-PULSE Seminar	Aug 30 th	2012
53.	Caught in the Act: Using stroboscopic measurements to study chemical dynamics		
	SLAC Colloquium	Jan 28 th	2013
54.	Ultrafast X-ray Laser Studies of Coupled Electronic and Nuclear Relaxation D		
	SLAC Photon Science Seminar	Mar 20 th	2013
55.	Ligand and Solvent Manipulation of Excited State Spin Dynamics in Iron Complex		
	ACS National Meeting, New Orleans	Apr 9 th	2013
56.	Ultrafast X-ray Laser Studies of Coupled Electronic and Nuclear Relaxation D		
	University of Kansas Chemistry Department Colloquium	Apr 19 th	2013
57.	Time-Resolved X-ray Applications in Chemistry	1 -	
0,,	Ultrafast X-ray Summer School	Jun 13 th	2013
58	Ultrafast X-ray laser Studies of Chemical Dynamics		2013
50.	Helmholtz Center Berlin Colloquium	June 25 th	2013
50	Caught in the Act: Time Resolved Investigations of Chemical Dynamics	June 23	2013
J.J.	XFEL School and Symposium Dinard, France	Sep 17 th	2013
60	Tracking Charge and Spin Dynamics in Iron Complexes with K-edge Fluorescence		
υU.	Dynamic Pathways in Multidimensional Landscapes Berlin, Germany	Sept 19 th	
	Dynamic Laurways in Municipilolial Laurscapes Dellin, Germany	Sept 19	2013

	Tracking Excited State Charge and Spin Dynamics in Iron Complexes University of Nevada-Reno Chemistry Department Colloquium	Apr 11 th	2014
62.	Ion Recognition and Assembly Dynamics in Aqueous Solution Telluride Science Research Center	Jul 8 th	2014
63.	Can we control electronic excited states in 3d coordination chemistry with ligand en	igineering	?
	Ultrafast Experiments at XFEL Sources Sørup Herregård, Denmark	Aug 25 th	2014
64.	Investigating Chemical Reaction Dynamics with Time Resolved X-ray Tools	_	
	Pico to Femto Helmholtz Zentrum Berlin	Jan 26th	2015
65.	Tracking the charge and spin dynamics of electronic excited states in inorganic con	nplexes	
	American Physical Society San Antonio, TX	Mar 2 nd	2015
66.	Site Specific Solvation Dynamics in Inorganic Chemistry		
	3 rd International Conference on Structural Dynamics Zurich, Switzerland	Jun 10 th	2015
67.	Probing Chemical Reaction Dynamics with Atomic Resolution and Specificity		
	XAFS16 Karlsruhe, Germany	Aug 25 th	2015
68.	Site Specific Solvation Dynamics of a Model Photocatalyst Studied with Ultrafast X	-ray Scatt	ering
	Pacificem Honolulu, HI	Dec 15 th	2015
69.	Making Molecular Movies: A New Era in X-ray Science		
	Board on Chemical Science & Technology, National Academy of Science Irvine CA	Aug 4th	2016
70.	Triangulating Intersections Between Electronic Excited States with Simultaneous	Ultrafast	X-ray
	Scattering and Spectroscopy		
	International Conference on Dynamic Pathways, Berlin, Germany	Sept 13 th	2016
71.	Femtosecond X-ray Laser Studies of Electron Transfer Dynamics in 3d Transition M	Aetal Com	plexes
	MIT School of Engineering	Dec 7 th	2016
72.	Triangulating Intersections Between Electronic Excited States with Simultaneous	Ultrafast	X-ray
	Scattering and Spectroscopy		•
	Banff 5 th Meeting on Structural Dynamics	Feb 19th	2017
73.	Addressing Persistent Challenges with Novel Tools: Ultrafast x-ray scattering prol	bes of liqu	id and
	solvation dynamics	•	
	ACS National Meeting San Francisco	Apr 2 nd	2017
74.	Ultrafast X-ray Laser Studies of Electronic Excited States in 3d Metal Complexes	•	
	ISPPCC Oxford, England	Jul 10 th	2017
75.	Finding Intersections Between Excited States with Ultrafast X-ray Scattering and S	pectrosco	ру
	Fontiers in Optics and Laser Science Washington D.C.	Sep18 th	2017
76.	Measuring Photo-Catalytic Reactions with Atomic Specificity and Chemical Accura	acy	
	Exascale Computing for Materials Genome Initiative Spetses Greece	Jun 12 th	2018
77.	Towards Control of Internal Conversion and Intersystem Crossoing in Iron Compl	exes	
	Time Resolved Chemistry Workshop, Argonne National Laboratory, IL	Oct 1st	2019
78.	Towards Control of 3d Transition Metal Complex Excited State Dynamics		
	Caltech Chemistry Seminar Pasadena, CA	Dec 9th	2019
79.	Developing the <i>ChemRIXS</i> Station: Chemical dynamics research at 120Hz		
	SSRL-LCLS Users Meeting	Sep 29th	2020
80.	Imaging Chemical Transformations with X-ray Lasers		
	University of Illinois at Champagne-Urbana Chemistry Seminar	Dec 2 nd	2020
81.	Imaging Chemical Transformations with X-ray Lasers		
	Imperial College, London Ultrafast Network Seminar	Dec 8 th	2021
82.	Accessing the Fluctuation Dynamics of Solutions with Ångström and Femtosecond	Resolution	1
	Pacifichem 2021 International Chemical Congress	Dec 16 th	2021
83.	Towards Control of Internal Conversion & Intersystem Crossing in Iron Coordina	tion Comp	lexes
	Pacifichem 2021 International Chemical Congress	Dec 17 th	2021
84.	Identifying Design Principles for Influencing Electronic Excited States of Metal Co		
	ACS National Meeting San Diego	Mar 24 th	2022
85.	Identifying Design Principles for Influencing Electronic Excited States of Metal Co	mplexes	
	Light-Controlled Reactivity in Metal Complexes, Jena, Germany	May 12 th	2022
86.	Capturing Chemical Dynamics with Atomic Specificity and Resolution		
	International Symposium on Molecular Spectroscopy, University of Illinois	Jun 20th	2023
87.	Capturing Photo-Driven Chemistry with Atomic Resolution and Specificity		
	Photochemistry Gordon Conference, Lewiston, Maine	Jul 30th	2023

Peer Reviewed Journal Articles

- 1. Femtosecond Dynamics of Electron Localization at Interfaces: N.-H. Ge, C.M. Wong, R.L. Lingle, Jr., J.D. McNeill, K.J. Gaffney, C.B. Harris, *Science* **279**, 202 (1998). *see also* Self-Trapping of Electrons at Surfaces: U. Hofer *Science* **279**, 190 (1998).
- 2. Femtosecond Studies of Electron Dynamics at Dielectric-Metal Interfaces: C.M. Wong, J.D. McNeill, K.J. Gaffney, N.-H. Ge, A.D. Miller, S.H. Liu, C.B. Harris, **feature article** *J. Phys. Chem. B* **103**, 282 (1999).
- 3. Femtosecond Electron Dynamics at the Benzene/Ag(111) Interface: K.J. Gaffney, C.M. Wong, S.H. Liu, A.D. Miller, J.D. McNeill, C.B. Harris, *Chem. Phys.* **251**, 99 (2000).
- The Adsorbate Electron Affinity Dependence of Femtosecond Electron Dynamics at Dielectric/Metal Interfaces: K.J. Gaffney, S.H. Liu, A.D. Miller, P. Szymanski, C.B. Harris, J. Chin. Chem. Soc. 47, 759 (2000).
- Femtosecond Dynamics of Electrons Photoinjected into Organic Semiconductors at Aromatic Metal Interfaces: K.J. Gaffney, A.D. Miller, S.H. Liu, C.B. Harris, feature article J. Phys. Chem. B 105, 9031 (2001).
- 6. Evolution of a Two Dimensional Band Structure at a Self-Assembling Interface: A.D. Miller, K.J. Gaffney, S.H. Liu, P. Szymanski, S. Garrett-Roe, C.B. Harris, *J. Phys. Chem.* A **106**, 7636 (2002).
- 7. Electron Solvation in Two Dimensions: A.D. Miller, I. Bezel, K.J. Gaffney, S. Garrett-Roe, S.H. Liu, P. Szymanski, C.B. Harris, *Science* **297**, 1163 (2002).
- 8. Hydrogen Bond Breaking and Reformation in Alcohol Oligomers Following Vibrational Relaxation of a Non-hydrogen Bond Donating Hydroxyl Stretch: K.J. Gaffney, I.R. Piletic, M.D. Fayer, *J. Phys. Chem. A* **106**, 9428 (2002).
- Direct Observation of Two Dimensional Electron Solvation By Alcohol/Ag(111) Interfaces: S.H. Liu, A.D. Miller, K.J. Gaffney, P. Szymanski, S. Garrett-Roe, I. Bezel, C.B. Harris, *J. Phys. Chem. B* 106, 12908 (2002).
- 10. Hydrogen Bond Dissociation and Reformation in Methanol Oligomers Following Hydroxyl Stretch Relaxation: K.J. Gaffney, P.H. Davis, N.E. Levinger, I.R. Piletic, M.D. Fayer, *J. Phys. Chem. A* **106**, 12012 (2002).
- 11. Orientational Relaxation and Vibrational Excitation Transfer in Methanol Carbon Tetrachloride Solutions: K.J. Gaffney, I.R. Piletic, M.D. Fayer, *J. Chem. Phys.* **118**, 2270 (2003).
- 12. Structural Dynamics of Hydrogen Bonded Methanol Oligomers: Vibrational Transient Hole Burning Studies of Spectral Diffusion: I.R. Piletic, K.J. Gaffney, M.D. Fayer, *J. Chem. Phys.* **119**, 423 (2003).
- 13. Ultrafast Heterodyne Detected Infrared Multidimensional Vibrational Stimulated Echo Studies of Hydrogen Bond Dynamics: J.B. Asbury, T. Steinel, C. Stromberg, K. J. Gaffney, I. R. Piletic, A. Goun, M. D. Fayer, *Chem. Phys. Lett.* **374**, 362 (2003).
- Hydrogen Bond Dynamics Probed with Ultrafast Infrared Heterodyne Detected Multidimensional Vibrational Stimulated Echoes: J.B. Asbury, T. Steinel, C. Stromberg, K. J. Gaffney, I. R. Piletic, A. Goun, M. D. Fayer, *Phys. Rev. Lett.* 91, 237402 (2003).
- 15. Hydrogen Bond Breaking Probed with Multidimensional Stimulated Vibrational Echo Correlation Spectroscopy: J.B. Asbury, T. Steinel, C. Stromberg, K.J. Gaffney, I.R. Piletic, M.D. Fayer, *J. Chem. Phys.* **119**, 12981 (2003).
- 16. Measurement and Dynamics of the Spatial Distribution of an Electron Localized at a Metal-Dielectric Interface: I. Bezel, K.J. Gaffney, S. Garrett-Roe, S.H. Liu, A.D. Miller, P. Szymanski, C.B. Harris, *J. Chem. Phys.* **120**, 845 (2004).
- 17. Clocking Femtosecond X-rays: A.L. Cavalieri et al., Phys. Rev. Lett. 94, 114801 (2005).
- 18. Atomic Scale Visualization of Inertial Dynamics: A.M. Lindenberg et al., Science 308, 392 (2005).
- 19. Observation of Structural Anisotropy and the Onset of Liquid-like Motion During the Nonthermal melting of InSb: K.J. Gaffney, *et al.*, *Phys. Rev. Lett.* **95**, 125701 (2005).
- 20. Ultrafast Dynamics of Laser-Excited Solids: D.A. Reis, K.J. Gaffney, G.H. Gilmer, D. Torralva, *Mat. Res. Soc. Bull.* **31**, 601 (2006).
- 21. Ultrafast Bond Softening in Bismuth: Mapping a Solid's Interatomic Potential with X-rays: D.M. Fritz, *et al. Science* **315**, 633 (2007). *see also* Watching Atoms Move: J.D. Brock *Science* 315, 609 (2007).
- 22. Carrier Density Dependent Lattice Stability in InSb: P.B. Hillyard, et al. Phys. Rev. Lett. 98, 125501 (2007).
- 23. Imaging Atomic Structure and Dynamics with Ultrafast X-ray Scattering: K.J. Gaffney, H.N. Chapman, *Science* **316**, 1444 (2007).
- 24. X-ray Diffuse Scattering Measurements of Nucleation Dynamics at Femtosecond Resolution: A.M. Lindenberg, *et al. Phys. Rev. Lett.* **100**, 135502 (2008).
- 25. Ultrafast Carrier Induced Disordering in InSb Studied with Density Functional Perturbation Theory: P.H. Hillyard, D.A. Reis, K.J. Gaffney, *Phys. Rev. B* 77, 195213 (2008).

- Efficient Multiple Exciton Generation Observed in Colloidal PbSe Quantum Dots with Temporally and Spectrally Resolved Intraband Excitation: M. Ji, S. Park, S.T. Connor, T. Mokari, Y. Cui, K.J. Gaffney, Nano. Lett. 9, 1217 (2009).
- 27. Ultrafast Dynamics of Hydrogen Bond Exchange in Aqueous Ionic Solutions: S. Park, M. Odelius, K.J. Gaffney, *J. Phys. Chem. B* **113**, 7825 (2009).
- 28. Atomic Resolution Mapping of the Excited State Electronic Structure of Cu₂O with Time-Resolved X-Ray Absorption Spectroscopy: P.B. Hillyard, *et al.*, *Phys. Rev. B* **80**, 125210 (2009).
- Characterization of Charge Transfer Excitations in Hexacyanomanganate(III) with Mn K-Edge Resonant Inelastic X-ray Scattering, D.A. Meyer, U. Bergmann, X. Zhang, K.J. Gaffney, *J. Chem. Phys.* 132, 134502 (2010).
- 30. Ligand Exchange Dynamics in Aqueous Solution Studied with 2DIR Spectroscopy: S. Park, M. Ji, K.J. Gaffney, *J. Phys. Chem. B* **114**, 6693 (2010).
- 31. Large Angular Jump Mechanism Observed for Hydrogen Bond Exchange in Aqueous Perchlorate Solution: M. Ji, M. Odelius, K.J. Gaffney, *Science* **328**, 1003 (2010). *see also* Following the Motions of Water Molecules in Aqueous Solutions: J.L. Skinner *Science* **328**, 985 (2010).
- 32. Dynamics of Ion Assembly in Solution: 2DIR Spectroscopy Study of LiNCS in Benzonitrile: M. Ji, S. Park, K.J. Gaffney, *J. Phys. Chem. Lett.* **1**, 1771 (2010).
- 33. Orientational Relaxation Dynamics in Aqueous Ionic Solution: Polarization-Selective Two-Dimensional Infrared Study of Angular Jump-Exchange Dynamics in Aqueous 6M NaClO₄: M. Ji, K.J. Gaffney, *J. Chem. Phys.* **134**, 044516 (2011).
- 34. H-bond Switching and Ligand Exchange Dynamics in Aqueous Ionic Solution: K.J. Gaffney, M. Ji, M. Odelius, S. Park, Z. Sun, **frontiers article** *Chem. Phys. Lett.* **504**, 1 (2011).
- 35. Characterizing the Deformational Isomers of Bimetallic Ir₂(dimen)₄²⁺ (dimen = 1,8-diisocyano-*p*-menthane) with Vibrational Wavepacket Dynamics: R.W. Hartsock, W. Zhang, M.G. Hill, B. Sabat, K.J. Gaffney, *J. Phys. Chem. A* **115**, 2920 (2011).
- 36. Interdependence of Conformational and Chemical Reaction Dynamics during Ion Assembly in Polar Solvents: M. Ji, R.W. Hartsock, Z. Sun, K.J. Gaffney, *J. Phys. Chem. B* **115**, 11399 (2011).
- 37. Direct Measurement of the Protein Response to an Electrostatic Perturbation that Mimics the Catalytic Cycle of Ketosteroid Isomerase: S.K. Jha, M. Ji, K.J. Gaffney, S.G. Boxer, *Proc. Natl. Acad. Sci. USA* **108**, 16612 (2011).
- 38. Influence of Solute-Solvent Coordination on the Orientational Relaxation of Ion Assemblies in Polar Solvents: M. Ji, R.W. Hartsock, Z. Sun, K.J. Gaffney, *J. Chem. Phys.* **136**, 014501 (2012).
- 39. Dynamics of Solvent Mediated Electron Localization in Electronically Excited Hexacyanoferrate(III): W. Zhang, M. Ji, Z. Sun, K.J. Gaffney, *J. Amer. Chem. Soc.* **134**, 2581 (2012).
- 40. Site-Specific Measurement of Water Dynamics in the Substrate Pocket of Ketosteroid Isomerase Using Time-Resolved Vibrational Spectroscopy: S.K. Jha, M. Ji, K.J. Gaffney, S.G. Boxer, *J. Phys. Chem. B* 116, 11414 (2012).
- 41. Resolving Photo-Induced Twisted Intramolecular Charge Transfer with Vibrational Anisotropy and TDDFT: W. Zhang, Z. Lan, Z. Sun, K.J. Gaffney, *J. Phys. Chem. B* **116**, 11527 (2012).
- 42. Resonant Inelastic Soft X-ray Scattering on Liquid Jets at Synchrotron and Free Electron Laser Light Sources: K. Kunnus, *et al. Rev. Sci. Instrum.***83**, 123109 (2012).
- 43. Femtosecond X-ray Absorption Spectroscopy at a Hard X-ray Free Electron Laser: Application to Spin Crossover Dynamics: H.T. Lemke, *et al. J. Phys. Chem. A* **117**, 735 (2013).
- 44. Aqueous Mg²⁺ and Ca²⁺ Ligand Exchange Mechanisms Identified with 2DIR Spectroscopy: Z. Sun, W. Zhang, M. Ji, and K.J. Gaffney, *J. Phys. Chem. B* **117**, 12268 (2013).
- 45. Contact Ion Pair Formation between Hard Acids and Soft Bases in Aqueous Solutions Observed with 2DIR Spectroscopy: Z. Sun, W. Zhang, M. Ji, R.W. Hartsock, K.J. Gaffney J. Phys. Chem. B 117, 15306 (2013).
- 46. Fourier-transform Inelastic X-ray Scattering from Time- and Momentum-Dependent Phonon-Phonon Correlations: M. Trigo, *et al. Nature Physics* **9**, 790 (2013). *see also* Condensed-matter physics: Picking up fine vibrations: P. Abbamonte *Nature Physics* **9**, 759 (2013).
- 47. Tracking Excited State Charge and Spin Dynamics in Iron Coordination Complexes: W. Zhang *et al. Nature* **509**, 345 (2014). *see also* X-ray spectroscopy: Enlightened state: J.K. McCusker *Nature Physics* **10**, 476 (2014).
- 48. Ultrafast X-ray Auger Probing of Photoexcited Molecular Dynamics: B.K. McFarland, et al. Nature Comm. 5, 4235 (2014).
- 49. Orbital-Specific Mapping of the Ligand Exchange Dynamics of Fe(CO)₅ in Solution: P. Wernet *et al. Nature* **520**, 78 (2015).
- 50. Mechanistic Studies of Photo-Induced Spin Crossover and Electron Transfer in Inorganic Complexes: W. Zhang, K.J. Gaffney *Acc. Chem. Res.* **48**, 1140 (2015).

- 51. Identification of the dominant photochemical pathways and mechanistic insights to the ultrafast ligand exchange of Fe(CO)₅ to Fe(CO)₄EtOH: K. Kunnus *et al. Struct. Dyn.* **3**, 043204 (2016).
- 52. Diffractive Imaging of a Molecular Rotational Wavepacket with Femtosecond Megaelectronvolt Electron Pulses: J. Yang, et al. *Nature Comm.* 7, 11232 (2016).
- 53. Femtosecond X-ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated [Co(terpy)₂]²⁺: E. Biasin, *et al. Phys. Rev. Lett.* **117**, 013002 (2016).
- 54. Viewing the Valence Electronic Structure of Ferric and Ferrous Hexacyanide in Solution from the Fe and Cyanide Perspectives: K. Kunnus, et al. J. Phys. Chem. B 120, 7182 (2016).
- 55. Anti-Stokes Resonant X-ray Raman Scattering for atom specific and excited state selective dynamics: K. Kunnus, *et al. New J. Phys.* **18**, 103011 (2016).
- 56. Atomistic Characterization of the Active-Site Solvation Dynamics of a Model Photocatalyst: T.B. van Driel, et. al. Nature Comm. 7, 13678 (2016).
- 57. Femtosecond Gas Phase Electron Diffraction with MeV Electrons: J. Yang, et al. Faraday Discuss. 194, 563 (2016).
- 58. Manipulating Charge Transfer Excited State Relaxation and Spin Crossover in Iron Coordination Complexes with Ligand Substitution: W. Zhang, et al. Chem. Sci. 8, 515 (2017).
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