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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

Chemical Sciences Division Director Energy Sciences Directorate, 2019-present
Deputy Associate Laboratory Director Energy Sciences Directorate, 2019-present
Associate Laboratory Director Stanford Synchrotron Radiation Lightsource, 2014-2019
Associate Professor Photon Science, SLAC, Stanford University, 2013-present
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

- Chair, Photon Science Department SLAC, Stanford University 2020-present
- Member, Advanced Photon Source Scientific Advisory Committee, 2020-present
- 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.
- Lead 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 Summer 2002
2. **Dynamics of Photoinjected Electrons at Model Molecular Electronic Interfaces**
Hewlett-Packard Lab Quantum Science Research Division May 9th 2003
3. **Time Resolving the Motions of Molecules at Surfaces and in Liquids**
SLAC Stanford Synchrotron Radiation Lab Jun 5th 2003
4. **Imaging Chemical Dynamics with Ultrafast X-rays**

	Stanford Linear Accelerator Center	SSRL 31 st User's Meeting	Oct 21 st	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	Aug 3 rd	2005
		Optics and Photonics National Meeting		
7.	Femtosecond X-ray Measurements of Structural Dynamics	Gordon Research Conference	Aug 9 th	2005
		X-ray Physics		
8.	Ultrafast X-ray Measurements of Structural Dynamics: technical challenges at the LCLS	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	SPIE Conference	May 9 th	2006
		High Power Laser Ablation 2006		
11.	Free electron laser studies of structural dynamics	Ultrafast Dynamics on Surfaces and in Liquids Workshop at SSRL	Oct 11 th	2006
12.	Ultrafast Diffuse Scattering Studies of Melting	SSRL User's Meeting	Oct 13 th	2006
13.	Making Molecular Movies: ten trillion frames per second	SLAC Public Lecture	Dec 12 th	2006
14.	Pump Probe Chemical Dynamics	Ultrafast X-ray Summer School at SLAC	Jun 20 th	2007
15.	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	American Chemical Society National Meeting	Apr 7 th	2008
17.	Experimental and theoretical studies of carrier dependent lattice stability in semiconductors	SPIE Conference	Apr 21 th	2008
		High Power Laser Ablation 2008		
18.	Making Molecular Movies	Low Energy Electrodynamics in Solids 2008	Jul 3 rd	2008
19.	X-ray Free Electron Laser Science	Stanford-Berkeley Synchrotron Summer School	Aug 21 th	2008
20.	Dynamics of Hydrogen Bond Exchange in Aqueous Electrolyte Solution	DOE Condensed Phase and Interfacial Molecular Science Meeting	Oct 21 th	2008
21.	Dynamics of Hydrogen Bond Exchange in Aqueous Electrolyte Solution	Argonne National Laboratory Chemistry Division Colloquium	Nov 11 th	2008
22.	Science Opportunities and Challenges at the X-ray Pump-Probe Endstation at the LCLS	JSSRR National Meeting	Jan 11 th	2009
		University of Tokyo		
23.	Science Opportunities and Challenges at the X-ray Pump-Probe Endstation at the LCLS	XFEL Colloquium at SPring-8	Jan 13 th	2009
24.	Dynamics of Hydrogen Bond Exchange in Aqueous Electrolyte Solution	Western Spectroscopy Association Meeting	Jan 29 th	2009
25.	Ionizing Radiation Induced Chemical Dynamics Studied with Ultrafast X-ray Lasers	Radiation Chemistry in the 21 st Century	Jul 13 th	2009
26.	Ionizing Radiation Induced Chemical Dynamics Studied with Ultrafast X-ray Lasers	6 th International Workshop on X-ray Radiation Damage	Mar 12 th	2010
27.	Non-equilibrium dynamics studied with femtosecond resolution X-ray scattering	PHONONS 2010	Apr 22 nd	2010
		National Taiwan University		
28.	Complex Molecules in Condensed Phases	Gordon Research Conference	Jul 22 nd	2010
		Atomic and Molecular Interactions		
29.	H-bond Switching and Ligand Exchange Dynamics in Aqueous Ionic Solution	CECAM Vibrational Spectroscopy of Complex Systems	May 23 rd	2011
30.	H-bond Switching and Ligand Exchange Dynamics in Aqueous Ionic Solution	Time Resolved Vibrational Spectroscopy XV	Jun 23 rd	2011
31.	How Does Water Solvate Ions?	Gordon Research Conference	Jun 28 th	2011
		Atomic Physics		
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 Ionic Solution**
University of Southern California Department of Chemistry Colloquium Nov 7th 2011
35. **Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous Ionic Solution**
University of California at Irvine Department of Chemistry Colloquium Nov 8th 2011
36. **Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous Ionic Solution**
University of Pennsylvania Department of Chemistry Colloquium Jan 19th 2012
37. **Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous Ionic Solution**
Colorado State University Department of Chemistry Colloquium Feb 2nd 2012
38. **Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous Ionic Solution**
University of Colorado Department of Chemistry Colloquium Feb 3rd 2012
39. **Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynamics**
Banff Meeting on Structural Dynamics Feb 21st 2012
40. **Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynamics**
American Physical Society March Meeting Feb 27th 2012
41. **Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous Ionic Solution**
MIT Department of Chemistry Colloquium Apr 10th 2012
42. **Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynamics**
Argonne Chemical Sciences Colloquium Apr 16th 2012
43. **Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous Ionic Solution**
University of Chicago Department of Chemistry Colloquium Apr 17th 2012
44. **Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous Ionic Solution**
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 Ionic Solution**
University of Wisconsin at Madison Department of Chemistry Colloquium Apr 20th 2012
46. **Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynamics**
Helmholtz Center Berlin Colloquium May 8th 2012
47. **Ultrafast X-ray laser Studies of Coupled Electronic and Nuclear Relaxation Dynamics**
Center for Free Electron Lasers May 9th 2012
48. **Vibrational Anisotropy Studies of Chemical Dynamics**
Max Born Institute Berlin May 11th 2012
49. **Resolving the Mechanism of H-bond Switching and Ligand Exchange in Aqueous Ionic Solution**
University of California at San Diego Department of Chemistry Colloquium May 22nd 2012
50. **Ion Recognition and Assembly: Mechanistic studies of ligand exchange in aqueous solution**
Telluride Science Research Center Jul 3rd 2012
51. **Tracking Non-Adiabatic Electron Transfer Dynamics with X-ray Spectroscopy**
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 30th 2012
53. **Caught in the Act: Using stroboscopic measurements to study chemical dynamics**
SLAC Colloquium Jan 28th 2013
54. **Ultrafast X-ray Laser Studies of Coupled Electronic and Nuclear Relaxation Dynamics**
SLAC Photon Science Seminar Mar 20th 2013
55. **Ligand and Solvent Manipulation of Excited State Spin Dynamics in Iron Complexes**
ACS National Meeting, New Orleans Apr 9th 2013
56. **Ultrafast X-ray Laser Studies of Coupled Electronic and Nuclear Relaxation Dynamics**
University of Kansas Chemistry Department Colloquium Apr 19th 2013
57. **Time-Resolved X-ray Applications in Chemistry**
Ultrafast X-ray Summer School Jun 13th 2013
58. **Ultrafast X-ray laser Studies of Chemical Dynamics**
Helmholtz Center Berlin Colloquium June 25th 2013
59. **Caught in the Act: Time Resolved Investigations of Chemical Dynamics**
XFEL School and Symposium Dinard, France Sep 17th 2013
60. **Tracking Charge and Spin Dynamics in Iron Complexes with K-edge Fluorescence Spectroscopy**
Dynamic Pathways in Multidimensional Landscapes Berlin, Germany Sept 19th 2013
61. **Tracking Excited State Charge and Spin Dynamics in Iron Complexes**
University of Nevada-Reno Chemistry Department Colloquium Apr 11th 2014
62. **Ion Recognition and Assembly Dynamics in Aqueous Solution**
Telluride Science Research Center Jul 8th 2014
63. **Can we control electronic excited states in 3d coordination chemistry with ligand engineering?**

- Ultrafast Experiments at XFEL Sources Sørup Herregård, Denmark Aug 25th 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 complexes**
American Physical Society San Antonio, TX Mar 2nd 2015
66. **Site Specific Solvation Dynamics in Inorganic Chemistry**
3rd International Conference on Structural Dynamics Zurich, Switzerland Jun 10th 2015
67. **Probing Chemical Reaction Dynamics with Atomic Resolution and Specificity**
XAFS16 Karlsruhe, Germany Aug 25th 2015
68. **Site Specific Solvation Dynamics of a Model Photocatalyst Studied with Ultrafast X-ray Scattering**
Pacificem Honolulu, HI Dec 15th 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 13th 2016
71. **Femtosecond X-ray Laser Studies of Electron Transfer Dynamics in 3d Transition Metal Complexes**
MIT School of Engineering Dec 7th 2016
72. **Triangulating Intersections Between Electronic Excited States with Simultaneous Ultrafast X-ray Scattering and Spectroscopy**
Banff 5th Meeting on Structural Dynamics Feb 19th 2017
73. **Addressing Persistent Challenges with Novel Tools: Ultrafast x-ray scattering probes of liquid and solvation dynamics**
ACS National Meeting San Francisco Apr 2nd 2017
74. **Ultrafast X-ray Laser Studies of Electronic Excited States in 3d Metal Complexes**
ISPPCC Oxford, England Jul 10th 2017
75. **Finding Intersections Between Excited States with Ultrafast X-ray Scattering and Spectroscopy**
Frontiers in Optics and Laser Science Washington D.C. Sep 18th 2017
76. **Measuring Photo-Catalytic Reactions with Atomic Specificity and Chemical Accuracy**
Exascale Computing for Materials Genome Initiative Spetses Greece Jun 12th 2018
77. **Towards Control of Internal Conversion and Intersystem Crossing in Iron Complexes**
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 ChemRIXS 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 2nd 2020

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).
4. 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).
5. 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).
9. 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).
14. 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 Disorder in InSb Studied with Density Functional Perturbation Theory: P.H. Hillyard, D.A. Reis, K.J. Gaffney, *Phys. Rev. B* **77**, 195213 (2008).
26. 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).
29. 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. Odellius, 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-diisocyno-*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).

59. Charge and Spin State Characterization of Cobalt Bis(*o*-Dioxolene) Valence Tautomers using Co K β X-ray Emission and L-edge X-ray Absorption Spectroscopies: H.W. Liang, *et al. Inorg. Chem.* **56**, 737 (2017).
60. Watching Coherent Molecular Structural Dynamics During Photoreaction: Beyond Kinetic Description: H.T. Lemke, *et al. Nature Comm.* **8**, 15342 (2017).
61. Ligand Manipulation of Charge Transfer Excited State Relaxation and Spin Crossover in [Fe(2,2'-bipyridine)₂(CN)₂]: K.S. Kjær, *et al. Struct. Dyn.* **4**, 044303 (2017).
62. Probing Ultrafast $\pi\pi^*/n\pi^*$ Internal Conversion in Organic Chromophores via K-edge Resonant Absorption: T.J.A. Wolf, *et al. Nature Comm.* **8**, 29 (2017).
63. Metalloprotein Control over Ligand-Metal Bonding Quantified by Femtosecond X-ray Spectroscopy: M.W. Mara *et al. Science* **356**, 1276 (2017). *see also* – Locked and Loaded for Apoptosis: K.L. Bren, E.L. Raven *Science* **356**, 1236 (2017).
64. L-Edge Spectroscopy of Dilute, Radiation-Sensitive Systems Using a Transition-Edge-Sensor Array: C.J. Titus, *et al. J. Chem. Phys.* **147**, 2314201 (2017).
65. Anisotropy Enhanced X-ray Scattering from Solvated Transition Metal Complexes: E. Biasin, *et al. J. Synch. Rad.* **25**, 306 (2018).
66. Solvent Control of Charge Transfer Excited State Relaxation Pathways in [Fe(2,2'-bipyridine)(CN)₄]²⁻: K.S. Kjær, *et al. Phys. Chem. Chem. Phys.* **20**, 4238 (2018).
67. Fingerprints of the Electronic, Spin and Structural Dynamics from Resonant Inelastic Soft X-ray Scattering in Transient Photo-Chemical Species: J. Norell, *et al. Phys. Chem. Chem. Phys.* **20**, 7243 (2018).
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