



Kelly Gaffney

Associate Professor of Photon Science and, by courtesy, of Chemistry

Photon Science Directorate

 Curriculum Vitae available Online

Bio

BIO

Professor Gaffney leads a research team focused on femtosecond resolution measurements of chemical dynamics in complex condensed phase systems. This research takes advantage of recent advances in ultrafast x-ray lasers, like the LCLS at SLAC National Accelerator Laboratory, to directly observe chemical reactions on the natural time and length scales of the chemical bond – femtoseconds and Ångströms. This research focuses on the discovery of design principles for controlling the non-equilibrium dynamics of electronic excited states and using these principles to spark new approaches to light-driven catalysis in chemical synthesis.

This research builds on Professor Gaffney's extensive experience with ultrafast optical laser science and technology. This work began with time- and angle- resolved two photon photoemission studies of electron solvation and localization at interfaces as a graduate student working with Professor Charles Harris at the University of California at Berkeley and extended to multidimensional vibrational spectroscopy studies of hydrogen bonding and ion solvation dynamics in solution during postdoctoral studies with Professor Michael Fayer at Stanford and as an Assistant Professor. The transition to ultrafast x-ray science began in 2004 at SLAC, where he helped establish the first chemical dynamics research program at SLAC.

ACADEMIC APPOINTMENTS

- Associate Professor, Photon Science Directorate
- Associate Professor (By courtesy), Chemistry

ADMINISTRATIVE APPOINTMENTS

- Department chair, Photon Science Department, (2020- present)
- Chemical Sciences Division Director, Energy Sciences Directorate, SLAC National Accelerator Laboratory, (2019- present)
- Deputy Associate Laboratory Director, Energy Sciences Directorate, SLAC National Accelerator Laboratory, (2019- present)
- Associate Laboratory Director, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, (2014-2019)
- Principle Investigator, PULSE Institute, (2007- present)

PROFESSIONAL EDUCATION

- PhD, University of California at Berkeley , Chemistry (2001)

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

The research team Professor Gaffney leads focuses on time resolved studies of chemical reactions. Recent advances in ultrafast x-ray lasers, like the LCLS at SLAC National Accelerator Laboratory, enable chemical reactions to be observed on the natural time and length scales of the chemical bond – femtoseconds and Ångströms. The knowledge gained from x-ray and optical laser studies will be used to spark new approaches to photo-catalysis and chemical synthesis.

Teaching

STANFORD ADVISEES

Postdoctoral Faculty Sponsor

Douglas Garratt, Alice Green, Wenhui Hu, Hyeongtaek Lim, Natalia Powers-Riggs, Sumana Raj, Elizabeth Ryland, Michael Sachs, Marija Zoric

Doctoral Dissertation Advisor (AC)

Shuri Francis, Kacie Nelson

Publications

PUBLICATIONS

- **Capturing Atom-Specific Electronic Structural Dynamics of Transition-Metal Complexes with Ultrafast Soft X-Ray Spectroscopy.** *Annual review of physical chemistry*
Jay, R. M., Kunnus, K., Wernet, P., Gaffney, K. J.
1800
- **Capturing photochemical and photophysical transformations in iron complexes with ultrafast X-ray spectroscopy and scattering** *CHEMICAL SCIENCE*
Gaffney, K. J.
2021; 12 (23): 8010-8025
- **Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer.** *Nature chemistry*
Biasin, E., Fox, Z. W., Andersen, A., Ledbetter, K., Kjar, K. S., Alonso-Mori, R., Carlstad, J. M., Chollet, M., Gaynor, J. D., Glowina, J. M., Hong, K., Kroll, T., Lee, et al
2021
- **Chemical control of competing electron transfer pathways in iron tetracyano-polypyridyl photosensitizers** *CHEMICAL SCIENCE*
Kunnus, K., Li, L., Titus, C., Lee, S., Reinhard, M. E., Koroidov, S., Kjaer, K. S., Hong, K., Ledbetter, K., Doriese, W. B., O'Neil, G. C., Swetz, D. S., Ullom, et al
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- **Atomistic characterization of the active-site solvation dynamics of a model photocatalyst** *NATURE COMMUNICATIONS*
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2016; 7
- **Large Angular Jump Mechanism Observed for Hydrogen Bond Exchange in Aqueous Perchlorate Solution** *SCIENCE*
Ji, M., Odelius, M., Gaffney, K. J.
2010; 328 (5981): 1003-1005
- **Quantifying the Steric Effect on Metal-Ligand Bonding in Fe Carbene Photosensitizers with Fe 2p3d Resonant Inelastic X-ray Scattering.** *Inorganic chemistry*
Kunnus, K., Guo, M., Biasin, E., Larsen, C. B., Titus, C. J., Lee, S. J., Nordlund, D., Cordones, A. A., Uhlig, J., Gaffney, K. J.
1800
- **Reduction of Electron Repulsion in Highly Covalent Fe-Amido Complexes Counteracts the Impact of a Weak Ligand Field on Excited-State Ordering.** *Journal of the American Chemical Society*
Larsen, C. B., Braun, J. D., Lozada, I. B., Kunnus, K., Biasin, E., Kolodziej, C., Burda, C., Cordones, A. A., Gaffney, K. J., Herbert, D. E.

2021

- **Direct observation of ultrafast hydrogen bond strengthening in liquid water.** *Nature*
Yang, J., Dettori, R., Nunes, J. P., List, N. H., Biasin, E., Centurion, M., Chen, Z., Cordones, A. A., Deponte, D. P., Heinz, T. F., Kozina, M. E., Ledbetter, K., Lin, et al
2021; 596 (7873): 531-535
- **Short-lived metal-centered excited state initiates iron-methionine photodissociation in ferrous cytochrome c.** *Nature communications*
Reinhard, M. E., Mara, M. W., Kroll, T., Lim, H., Hadt, R. G., Alonso-Mori, R., Chollet, M., Glowonia, J. M., Nelson, S., Sokaras, D., Kunnus, K., Driel, T. B., Hartsock, et al
2021; 12 (1): 1086
- **Photodissociation of aqueous I3- observed with liquid-phase ultrafast mega-electronvolt electron diffraction** *Structural Dynamics*
Ledbetter, K., et al
2020; 21: 10
- **Origin of core-to-core x-ray emission spectroscopy sensitivity to structural dynamics.** *Structural dynamics (Melville, N.Y.)*
Vacher, M., Kunnus, K., Delcey, M. G., Gaffney, K. J., Lundberg, M.
2020; 7 (4): 044102
- **XFELs: cutting edge X-ray light for chemical and material sciences** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
Asakura, K., Gaffney, K. J., Milne, C., Yabashi, M.
2020; 22 (5): 2612-14
- **Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering.** *Nature communications*
Kunnus, K., Vacher, M., Harlang, T. C., Kjar, K. S., Haldrup, K., Biasin, E., van Driel, T. B., Papai, M., Chabera, P., Liu, Y., Tatsuno, H., Timm, C., Kallman, et al
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- **Simulations of valence excited states in coordination complexes reached through hard X-ray scattering.** *Physical chemistry chemical physics : PCCP*
Källman, E. n., Guo, M. n., Delcey, M. G., Meyer, D. A., Gaffney, K. J., Lindh, R. n., Lundberg, M. n.
2020; 22 (16): 8325-35
- **Femtosecond electronic structure response to high intensity XFEL pulses probed by iron X-ray emission spectroscopy.** *Scientific reports*
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2020; 10 (1): 16837
- **Excited state charge distribution and bond expansion of ferrous complexes observed with femtosecond valence-to-core x-ray emission spectroscopy** *Journal of Chemical Physics*
Ledbetter, K., Reinhard, M. E., Kunnus, K., Gallo, A., Britz, A., Biasin, E., Glowonia, J. M., Nelson, S., Van Driel, T. B., Weninger, C., Zederkof, D. B., Haldrup, K., Cordones, et al
2020; 152
- **Finding intersections between electronic excited state potential energy surfaces with simultaneous ultrafast X-ray scattering and spectroscopy.** *Chemical science*
Kjar, K. S., Van Driel, T. B., Harlang, T. C., Kunnus, K., Biasin, E., Ledbetter, K., Hartsock, R. W., Reinhard, M. E., Koroidov, S., Li, L., Laursen, M. G., Hansen, F. B., Vester, et al
2019; 10 (22): 5749-60
- **Ultrafast X-Ray Scattering Measurements of Coherent Structural Dynamics on the Ground-State Potential Energy Surface of a Diplatinum Molecule** *PHYSICAL REVIEW LETTERS*
Haldrup, K., Levi, G., Biasin, E., Vester, P., Laursen, M., Beyer, F., Kjaer, K., van Driel, T., Harlang, T., Dohn, A. O., Hartsock, R. J., Nelson, S., Glowonia, et al
2019; 122 (6): 063001
- **Initial metal-metal bond breakage detected by fs X-ray scattering in the photolysis of Ru-3(CO)(12) in cyclohexane at 400 nm** *PHOTOCHEMICAL & PHOTOBIOLOGICAL SCIENCES*
Kong, Q. Y., Laursen, M. G., Haldrup, K., Kjaer, K. S., Khakhulin, D., Biasin, E., van Driel, T. B., Wulff, M., Kabanova, V., Vuilleumier, R., Bratos, S., Nielsen, M. M., Gaffney, et al
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- **Soft X-ray spectroscopy with transition-edge sensors at Stanford Synchrotron Radiation Lightsource beamline 10-1** *Review of Scientific Instruments*

- Lee, S., Titus, C. J., Alonso-Mori, R., Baker, M. L., Bennett, D. A., Cho, H., Doriese, W. B., Fowler, J. W., Gaffney, K. J., Gallo, A., Gard, J. D., Hilton, G. C., Jang, et al
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- **Hot Branching Dynamics in a Light-Harvesting Iron Carbene Complex Revealed by Ultrafast X-ray Emission Spectroscopy.** *Angewandte Chemie (International ed. in English)*
Tatsuno, H. n., Kjaer, K. S., Kunnus, K. n., Harlang, T. C., Timm, C. n., Guo, M. n., Chàbera, P. n., Fredin, L. A., Hartsock, R. W., Reinhard, M. E., Koroidov, S. n., Li, L. n., Cordones, et al
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 - **Probing the Electron Accepting Orbitals of Ni-Centered Hydrogen Evolution Catalysts with Noninnocent Ligands by Ni L-Edge and S K-Edge X-ray Absorption** *INORGANIC CHEMISTRY*
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2018; 57 (21): 13167–75
 - **Disentangling Transient Charge Density and Metal-Ligand Covalency in Photoexcited Ferricyanide with Femtosecond Resonant Inelastic Soft X-ray Scattering** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
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 - **Fingerprints of electronic, spin and structural dynamics from resonant inelastic soft X-ray scattering in transient photo-chemical species** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
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2018; 20 (10): 7243–53
 - **Anisotropy enhanced X-ray scattering from solvated transition metal complexes** *JOURNAL OF SYNCHROTRON RADIATION*
Biasin, E., van Driel, T. B., Levi, G., Laursen, M. G., Dohn, A. O., Moltke, A., Vester, P., Hansen, F. K., Kjaer, K. S., Harlang, T., Hartsock, R., Christensen, M., Gaffney, et al
2018; 25: 306–15
 - **Solvent control of charge transfer excited state relaxation pathways in [Fe(2,2'-bipyridine)(CN)(4)](2-)** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
Kjaer, K. S., Kunnus, K., Harlang, T. B., Van Driel, T. B., Ledbetter, K., Hartsock, R. W., Reinhard, M. E., Koroidov, S., Li, L., Laursen, M. G., Biasin, E., Hansen, F. B., Vester, et al
2018; 20 (6): 4238–49
 - **L-edge spectroscopy of dilute, radiation-sensitive systems using a transition-edge-sensor array** *JOURNAL OF CHEMICAL PHYSICS*
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2017; 147 (21): 214201
 - **Ligand manipulation of charge transfer excited state relaxation and spin crossover in [Fe(2,2'-bipyridine)(2)(CN)(2)]** *STRUCTURAL DYNAMICS*
Kjaer, K. S., Zhang, W., Alonso-Mori, R., Bergmann, U., Chollet, M., Hadt, R. G., Hartsock, R. W., Harlang, T., Kröll, T., Kubicek, K., Lemke, H. T., Liang, H. W., Liu, et al
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 - **Metalloprotein entatic control of ligand-metal bonds quantified by ultrafast x-ray spectroscopy** *SCIENCE*
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 - **Probing ultrafast pi pi*/n pi* internal conversion in organic chromophores via K-edge resonant absorption** *NATURE COMMUNICATIONS*
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2017; 8: 29
 - **Coherent structural trapping through wave packet dispersion during photoinduced spin state switching** *NATURE COMMUNICATIONS*
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Liang, H. W., Kroll, T., Nordlund, D., Weng, T., Sokaras, D., Pierpont, C. G., Gaffney, K. J.
2017; 56 (2): 737-747
- **Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution** *CHEMICAL SCIENCE*
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- **Anti-Stokes resonant x-ray Raman scattering for atom specific and excited state selective dynamics** *NEW JOURNAL OF PHYSICS*
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2016; 18
- **Viewing the Valence Electronic Structure of Ferric and Ferrous Hexacyanide in Solution from the Fe and Cyanide Perspectives** *JOURNAL OF PHYSICAL CHEMISTRY B*
Kunnus, K., Zhang, W., Delcey, M. G., Pinjari, R. V., Miedema, P. S., Schreck, S., Quevedo, W., Schroeder, H., Foehlich, A., Gaffney, K. J., Lundberg, M., Odelius, M., Wernet, et al
2016; 120 (29): 7182-7194
- **Identification of the dominant photochemical pathways and mechanistic insights to the ultrafast ligand exchange of Fe(CO)5 to Fe(CO)4EtOH.** *Structural dynamics*
Kunnus, K., JOSEFSSON, I., RAJKOVIC, I., Schreck, S., Quevedo, W., Beye, M., Weniger, C., Grübel, S., Scholz, M., Nordlund, D., Zhang, W., Hartsock, R. W., Gaffney, et al
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- **Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated [Co(terpy)(2)](2+)** *PHYSICAL REVIEW LETTERS*
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- **Diffraction imaging of a rotational wavepacket in nitrogen molecules with femtosecond megaelectronvolt electron pulses** *NATURE COMMUNICATIONS*
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- **Femtosecond gas phase electron diffraction with MeV electrons** *FARADAY DISCUSSIONS*
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- **Orbital-specific mapping of the ligand exchange dynamics of Fe(CO)(5) in solution** *NATURE*
Wernet, P., Kunnus, K., JOSEFSSON, I., RAJKOVIC, I., Quevedo, W., Beye, M., Schreck, S., Gruebel, S., Scholz, M., Nordlund, D., Zhang, W., Hartsock, R. W., Schlotter, et al
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Zhang, W., Gaffney, K. J.
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- **Ultrafast X-ray Auger probing of photoexcited molecular dynamics** *NATURE COMMUNICATIONS*
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- **Fourier-transform inelastic X-ray scattering from time- and momentum-dependent phonon-phonon correlations** *NATURE PHYSICS*
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- **Aqueous Mg(2+) and Ca(2+) Ligand Exchange Mechanisms Identified with 2DIR Spectroscopy.** *journal of physical chemistry. B*
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- **Site-Specific Measurement of Water Dynamics in the Substrate Pocket of Ketosteroid Isomerase Using Time-Resolved Vibrational Spectroscopy** *JOURNAL OF PHYSICAL CHEMISTRY B*
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- **Resolving Photo-Induced Twisted Intramolecular Charge Transfer with Vibrational Anisotropy and TDDFT** *JOURNAL OF PHYSICAL CHEMISTRY B*
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- **Interdependence of Conformational and Chemical Reaction Dynamics during Ion Assembly in Polar Solvents** *JOURNAL OF PHYSICAL CHEMISTRY B*
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- **Orientational relaxation dynamics in aqueous ionic solution: Polarization-selective two-dimensional infrared study of angular jump-exchange dynamics in aqueous 6M NaClO4** *JOURNAL OF CHEMICAL PHYSICS*
Ji, M., Gaffney, K. J.
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- **Ligand Exchange Dynamics in Aqueous Solution Studied with 2DIR Spectroscopy** *JOURNAL OF PHYSICAL CHEMISTRY B*
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- **Characterization of charge transfer excitations in hexacyanomanganate(III) with Mn K-edge resonant inelastic x-ray scattering** *JOURNAL OF CHEMICAL PHYSICS*
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Lindenberg, A. M., Engemann, S., Gaffney, K. J., Sokolowski-Tinten, K., Larsson, J., Hillyard, P. B., Reis, D. A., Fritz, D. M., ARTHUR, J., Akre, R. A., George, M. J., Deb, A., Bucksbaum, et al
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