

Stanford



Kelly Gaffney

Professor of Photon Science

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

- Professor, Photon Science Directorate

ADMINISTRATIVE APPOINTMENTS

- Interim Associate Laboratory Director, Energy Sciences Directorate, SLAC National Accelerator Laboratory, (2023- present)
- Department chair, Photon Science Department, (2020-2023)
- Chemical Sciences Division Director, Energy Sciences Directorate, SLAC National Accelerator Laboratory, (2019-2023)
- Deputy Associate Laboratory Director, Energy Sciences Directorate, SLAC National Accelerator Laboratory, (2019-2023)
- 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

Doctoral Dissertation Reader (AC)

Andy Mitchell

Postdoctoral Faculty Sponsor

Hao Chen, Yukio Cho, Alice Green, Reagan Hooper, Tom Hopper, Wenhui Hu, Philipp Lenzen, Hyeongtaek Lim, Cheolwoo Park, Ben Poulter, Elizabeth Ryland, Michael Sachs

Doctoral Dissertation Advisor (AC)

Shuri Francis, Kacie Nelson

Publications

PUBLICATIONS

- **Optically Induced Anisotropy in Time-Resolved Scattering: Imaging Molecular-Scale Structure and Dynamics in Disordered Media with Experiment and Theory.** *Physical review letters*
Montoya-Castillo, A., Chen, M. S., Raj, S. L., Jung, K. A., Kjaer, K. S., Morawietz, T., Gaffney, K. J., van Driel, T. B., Markland, T. E.
2022; 129 (5): 056001
- **Capturing Atom-Specific Electronic Structural Dynamics of Transition-Metal Complexes with Ultrafast Soft X-Ray Spectroscopy.** *Annual review of physical chemistry*
Jay, R. M., Kunus, K., Wernet, P., 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., Kunus, K., Biasin, E., Kolodziej, C., Burda, C., Cordones, A. A., Gaffney, K. J., Herbert, D. E.
2021
- **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
- **Chemical control of competing electron transfer pathways in iron tetracyano-polypyridyl photosensitizers** *CHEMICAL SCIENCE*
Kunus, K., Li, L., Titus, C., Lee, S., Reinhard, M. E., Koroidov, S., Kjaer, K. S., Hong, K., Ledbetter, K., Dorise, W. B., O'Neil, G. C., Swetz, D. S., Ullom, et al
2020; 11 (17): 4360–73
- **Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering.** *Nature communications*
Kunus, 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
2020; 11 (1): 634
- **Solution phase high repetition rate laser pump x-ray probe picosecond hard x-ray spectroscopy at the Stanford Synchrotron Radiation Lightsource** *STRUCTURAL DYNAMICS-US*
Reinhard, M., Skoien, D., Spies, J. A., Garcia-Esparza, A. T., Matson, B. D., Corbett, J., Tian, K., Safranek, J., Granados, E., Strader, M., Gaffney, K. J., Alonso-Mori, R., Kroll, et al

2023; 10 (5): 054304

● **Ferricyanide photo-aquation pathway revealed by combined femtosecond K# main line and valence-to-core x-ray emission spectroscopy.** *Nature communications*

Reinhard, M., Gallo, A., Guo, M., Garcia-Esparza, A. T., Biasin, E., Qureshi, M., Britz, A., Ledbetter, K., Kunnus, K., Weninger, C., van Driel, T., Robinson, J., Glownia, et al
2023; 14 (1): 2443

● **Dissociation of Pyridinethiolate Ligands during Hydrogen Evolution Reactions of Ni-Based Catalysts: Evidence from X-ray Absorption Spectroscopy.** *Inorganic chemistry*

Ledbetter, K., Larsen, C. B., Lim, H., Zoric, M. R., Koroidov, S., Pemmaraju, C. D., Gaffney, K. J., Cordones, A. A.
2022

● **The case for data science in experimental chemistry: examples and recommendations** *NATURE REVIEWS CHEMISTRY*

Yano, J., Gaffney, K. J., Gregoire, J., Hung, L., Ourmazd, A., Schrier, J., Sethian, J. A., Toma, F. M.
2022; 6 (5): 357-370

● **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

● **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

● **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., Glownia, J. M., Hong, K., Kroll, T., Lee, et al
2021

● **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., Glownia, 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

● **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*

Alonso-Mori, R. n., Sokaras, D. n., Cammarata, M. n., Ding, Y. n., Feng, Y. n., Fritz, D. n., Gaffney, K. J., Hastings, J. n., Kao, C. C., Lemke, H. T., Maxwell, T. n., Robert, A. n., Schropp, et al
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., Glownia, 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., Glownia, 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
2019; 18 (2): 319–27

• **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
2019

• **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
2019; 90

• **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*

Koroidov, S., Hong, K., Kjaer, K. S., Li, L., Kunnus, K., Reinhard, M., Hartsock, R. W., Amit, D., Eisenberg, R., Das Pemmaraju, C., Gaffney, K. J., Cordones, A. A.
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*

Jay, R. M., Norell, J., Eckert, S., Hantschmann, M., Beye, M., Kennedy, B., Quevedo, W., Schlotter, W. F., Dakovski, G. L., Miniti, M. P., Hoffmann, M. C., Mitra, A., Moeller, et al
2018; 9 (12): 3538–43

• **Fingerprints of electronic, spin and structural dynamics from resonant inelastic soft X-ray scattering in transient photo-chemical species** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*

Norell, J., Jay, R. M., Hantschmann, M., Eckert, S., Guo, M., Gaffney, K. J., Wernet, P., Lundberg, M., Foehlisch, A., Odelius, M.
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*

Titus, C. J., Baker, M. L., Lee, S., Cho, H., Doriese, W. B., Fowler, J. W., Gaffney, K., Gard, J. D., Hilton, G. C., Kenney, C., Knight, J., Li, D., Marks, et al
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., Kroll, T., Kubicek, K., Lemke, H. T., Liang, H. W., Liu, et al
2017; 4 (4): 044030

- **Metalloprotein entatic control of ligand-metal bonds quantified by ultrafast x-ray spectroscopy** *SCIENCE*
Mara, M. W., Hadt, R. G., Reinhard, M., Kroll, T., Lim, H., Hartsock, R. W., Alonso-Mori, R., Chollet, M., Glownia, J. M., Nelson, S., Sokaras, D., Kunnus, K., Hodgson, et al
2017; 356 (6344): 1276+
- **Probing ultrafast pi pi*/n pi* internal conversion in organic chromophores via K-edge resonant absorption** *NATURE COMMUNICATIONS*
Wolf, T. A., Myhre, R. H., Cryan, J. P., Coriani, S., Squibb, R. J., Battistoni, A., Berrah, N., Bostedt, C., Bucksbaum, P., Coslovich, G., Feifel, R., Gaffney, K. J., Grilj, et al
2017; 8: 29
- **Coherent structural trapping through wave packet dispersion during photoinduced spin state switching** *NATURE COMMUNICATIONS*
Lemke, H. T., Kjaer, K. S., Hartsock, R., van Driel, T. B., Chollet, M., Glownia, J. M., Song, S., Zhu, D., Pace, E., Matar, S. F., Nielsen, M. M., Benfatto, M., Gaffney, et al
2017; 8
- **Charge and Spin-State Characterization of Cobalt Bis(o-dioxolene) Valence Tautomers Using Co K beta X-ray Emission and L-Edge X-ray Absorption Spectroscopies** *INORGANIC CHEMISTRY*
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*
Zhang, W., Kjaer, K. S., Alonso-Mori, R., Bergmann, U., Chollet, M., Fredin, L. A., Hadt, R. G., Hartsock, R. W., Harlang, T., Kroll, T., Kubicek, K., Lemke, H. T., Liang, et al
2017; 8 (1): 515-523
- **Atomistic characterization of the active-site solvation dynamics of a model photocatalyst** *NATURE COMMUNICATIONS*
van Driel, T. B., Kjaer, K. S., Hartsock, R. W., Dohn, A. O., Harlang, T., Chollet, M., Christensen, M., Gawelda, W., Henriksen, N. E., Kim, J. G., Haldrup, K., Kim, K. H., Ihhee, et al
2016; 7
- **Anti-Stokes resonant x-ray Raman scattering for atom specific and excited state selective dynamics** *NEW JOURNAL OF PHYSICS*
Kunnus, K., Josefsson, I., Rajkovic, I., Schreck, S., Quevedo, W., Beye, M., Greubel, S., Scholz, M., Nordlund, D., Zhang, W., Hartsock, R. W., Gaffney, K. J., Schlotter, et al
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., Foehlisch, 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
2016; 3 (4): 043204-
- **Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated [Co(terpy)(2)](2+)** *PHYSICAL REVIEW LETTERS*
Biasin, E., van Driel, T., Kjaer, K. S., Dohn, A. O., Christensen, M., Harlang, T., Chabera, P., Liu, Y., Uhlig, J., Papai, M., Nemeth, Z., Hartsock, R., Liang, et al
2016; 117 (1): 013002
- **Diffractive imaging of a rotational wavepacket in nitrogen molecules with femtosecond megaelectronvolt electron pulses** *NATURE COMMUNICATIONS*
Yang, J., Guehr, M., Vecchione, T., Robinson, M. S., Li, R., Hartmann, N., Shen, X., Coffee, R., Corbett, J., Fry, A., Gaffney, K., Gorkhover, T., Hast, et al
2016; 7
- **Femtosecond gas phase electron diffraction with MeV electrons** *FARADAY DISCUSSIONS*
Yang, J., Guehr, M., Vecchione, T., Robinson, M. S., Li, R., Hartmann, N., Shen, X., Coffee, R., Corbett, J., Fry, A., Gaffney, K., Gorkhover, T., Hast, et al
2016; 194: 563–81
- **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
2015; 520 (7545): 78-81

● **Mechanistic Studies of Photoinduced Spin Crossover and Electron Transfer in Inorganic Complexes** *ACCOUNTS OF CHEMICAL RESEARCH*

Zhang, W., Gaffney, K. J.
2015; 48 (4): 1140-1148

● **Ultrafast X-ray Auger probing of photoexcited molecular dynamics** *NATURE COMMUNICATIONS*

McFarland, B. K., Farrell, J. P., Miyabe, S., Tarantelli, F., Aguilar, A., Berrah, N., Bostedt, C., Bozek, J. D., Bucksbaum, P. H., Castagna, J. C., Coffee, R. N., Cryan, J. P., Fang, et al
2014; 5

● **Tracking excited-state charge and spin dynamics in iron coordination complexes.** *Nature*

Zhang, W., Alonso-Mori, R., Bergmann, U., Bressler, C., Chollet, M., Galler, A., Gawelda, W., Hadt, R. G., Hartsock, R. W., Kroll, T., Kjær, K. S., Kubicek, K., Lemke, et al
2014; 509 (7500): 345-348

● **Contact Ion Pair Formation between Hard Acids and Soft Bases in Aqueous Solutions Observed with 2DIR Spectroscopy** *JOURNAL OF PHYSICAL CHEMISTRY B*

Sun, Z., Zhang, W., Ji, M., Hartsock, R., Gaffney, K. J.
2013; 117 (49): 15306-15312

● **Fourier-transform inelastic X-ray scattering from time- and momentum-dependent phonon-phonon correlations** *NATURE PHYSICS*

Trigo, M., Fuchs, M., Chen, J., Jiang, M. P., Cammarata, M., Fahy, S., Fritz, D. M., Gaffney, K., Ghimire, S., Higginbotham, A., Johnson, S. L., Kozina, M. E., Larsson, et al
2013; 9 (12): 790-794

● **Aqueous Mg(2+) and Ca(2+) Ligand Exchange Mechanisms Identified with 2DIR Spectroscopy.** *journal of physical chemistry. B*

Sun, Z., Zhang, W., Ji, M., Hartsock, R., Gaffney, K. J.
2013; 117 (40): 12268-12275

● **Femtosecond X-ray Absorption Spectroscopy at a Hard X-ray Free Electron Laser: Application to Spin Crossover Dynamics** *JOURNAL OF PHYSICAL CHEMISTRY A*

Lemke, H. T., Bressler, C., Chen, L. X., Fritz, D. M., Gaffney, K. J., Galler, A., Gawelda, W., Haldrup, K., Hartsock, R. W., Ihée, H., Kim, J., Kim, K., Lee, et al
2013; 117 (4): 735–40

● **A setup for resonant inelastic soft x-ray scattering on liquids at free electron laser light sources** *REVIEW OF SCIENTIFIC INSTRUMENTS*

Kunnus, K., Rajkovic, I., Schreck, S., Quevedo, W., Eckert, S., Beye, M., Suljoti, E., Weniger, C., Kalus, C., Gruebel, S., Scholz, M., Nordlund, D., Zhang, et al
2012; 83 (12)

● **Resolving Photo-Induced Twisted Intramolecular Charge Transfer with Vibrational Anisotropy and TDDFT** *JOURNAL OF PHYSICAL CHEMISTRY B*

Zhang, W., Lan, Z., Sun, Z., Gaffney, K. J.
2012; 116 (37): 11527-11536

● **Site-Specific Measurement of Water Dynamics in the Substrate Pocket of Ketosteroid Isomerase Using Time-Resolved Vibrational Spectroscopy** *JOURNAL OF PHYSICAL CHEMISTRY B*

Jha, S. K., Ji, M., Gaffney, K. J., Boxer, S. G.
2012; 116 (37): 11414-11421

● **Dynamics of Solvent-Mediated Electron Localization in Electronically Excited Hexacyanoferrate(III)** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

Zhang, W., Ji, M., Sun, Z., Gaffney, K. J.
2012; 134 (5): 2581-2588

● **Influence of solute-solvent coordination on the orientational relaxation of ion assemblies in polar solvents** *JOURNAL OF CHEMICAL PHYSICS*

Ji, M., Hartsock, R. W., Sung, Z., Gaffney, K. J.
2012; 136 (1)

● **Interdependence of Conformational and Chemical Reaction Dynamics during Ion Assembly in Polar Solvents** *JOURNAL OF PHYSICAL CHEMISTRY B*

Ji, M., Hartsock, R. W., Sun, Z., Gaffney, K. J.

2011; 115 (39): 11399-11408

- **Direct measurement of the protein response to an electrostatic perturbation that mimics the catalytic cycle in ketosteroid isomerase** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

Jha, S. K., Ji, M., Gaffney, K. J., Boxer, S. G.

2011; 108 (40): 16612-16617

- **Characterizing the Deformational Isomers of Bimetallic Ir-2(dimen)(4)(2+)** (dimen=1,8-diisocyano-p-menthane) *with Vibrational Wavepacket Dynamics* *JOURNAL OF PHYSICAL CHEMISTRY A*

Hartsock, R. W., Zhang, W., Hill, M. G., Sabat, B., Gaffney, K. J.

2011; 115 (14): 2920-2926

- **H-bond switching and ligand exchange dynamics in aqueous ionic solution** *CHEMICAL PHYSICS LETTERS*

Gaffney, K. J., Ji, M., Odelius, M., Park, S., Sun, Z.

2011; 504 (1-3): 1-6

- **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.

2011; 134 (4)

- **Dynamics of Ion Assembly in Solution: 2DIR Spectroscopy Study of LiNCS in Benzonitrile** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*

Ji, M., Park, S., Gaffney, K. J.

2010; 1 (12): 1771-1775

- **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

- **Ligand Exchange Dynamics in Aqueous Solution Studied with 2DIR Spectroscopy** *JOURNAL OF PHYSICAL CHEMISTRY B*

Park, S., Ji, M., Gaffney, K. J.

2010; 114 (19): 6693-6702

- **Characterization of charge transfer excitations in hexacyanomanganate(III) with Mn K-edge resonant inelastic x-ray scattering** *JOURNAL OF CHEMICAL PHYSICS*

Meyer, D. A., Zhang, X., Bergmann, U., Gaffney, K. J.

2010; 132 (13)

- **Atomic resolution mapping of the excited-state electronic structure of Cu₂O with time-resolved x-ray absorption spectroscopy** *PHYSICAL REVIEW B*

Hillyard, P. W., Kuchibhatla, S. V., Glover, T. E., Hertlein, M. P., Huse, N., Nachimuthu, P., Saraf, L. V., Thevuthasan, S., Gaffney, K. J.

2009; 80 (12)

- **Ultrafast Dynamics of Hydrogen Bond Exchange in Aqueous Ionic Solutions** *JOURNAL OF PHYSICAL CHEMISTRY B*

Park, S., Odelius, M., Gaffney, K. J.

2009; 113 (22): 7825-7835

- **Efficient Multiple Exciton Generation Observed in Colloidal PbSe Quantum Dots with Temporally and Spectrally Resolved Intraband Excitation** *NANO LETTERS*

Ji, M., Park, S., Connor, S. T., Mokari, T., Cui, Y., Gaffney, K. J.

2009; 9 (3): 1217-1222

- **Carrier-induced disordering dynamics in InSb studied with density functional perturbation theory** *PHYSICAL REVIEW B*

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