Stanford



Gee, Leland B.

Staff Scientist, LCLS - Linac Coherent Light Source

Bio

BIO

Skills in spectroscopy with numerous spectroscopic techniques: Fourier-transform infrared spectroscopy, electron paramagnetic resonance, Fe-57 Mössbauer spectroscopy, X-ray magnetic circular dichroism, Ni-61 Mössbauer spectroscopy, XAS, XES, RIXS, EXAFS, and nuclear resonance vibrational spectroscopy. With a special focus on applying these approaches to bioinorganic systems.

Launched a website in 2015 called www.spectra.tools, aimed to make a repository of web-driven spectroscopy tools and information. With the hope that these spectroscopic methods and computational tools become more accessible to others.

Research interests currently include: Design of artificial metalloenzymes for gas transformation chemistry; photochemistry of nitric-oxide release from transition metals toward biomedical applications; and applications of advanced learning towards X-ray spectroscopy.

CURRENT ROLE AT STANFORD

The lead instrument scientist for the MFX instrument at the LCLS (at the SLAC National Accelerator Laboratory). Coordinator of the Bioinorganic Research Group with membership that spans multiple directorates at SLAC. Leader of an HPC project at NERSC to increase accessibility to the analysis of spectroscopic data, XSIM: "Computational simulations of advanced X-ray spectroscopy on biological metallocofactors".

Member of the NIH P41 Center for Structural Dynamics in Biology.

HONORS AND AWARDS

- Educational Committee Travel Award, Biophysical Society (2016)
- Graduate Student Research Award, UC Davis and Humanities (2015)
- Mössbauer Young Scientist Award, International Board on the Applications of the Mössbauer Effect (9/9/2021)

EDUCATION AND CERTIFICATIONS

- Ph.D., University of California, Davis , Biophysics (2016)
- B.S., University of California, Davis , Biochemistry/Molecular Biology (2011)
- B.A., University of California, Davis , Economics (2011)

PROJECTS

- Development of Photosynthetic Methane and Hydrogen Transforming Biohybrid Platforms
- Photomechanistic insights into NO- and HNO-evolving redox non-innocent metal-nitrosyl complexes

LINKS

- spectra.tools: https://www.spectra.tools
- Google Scholar: https://scholar.google.com/citations?hl=en&user=ICFW4MAAAAAJ&view_op=list_works&sortby=pubdate
- ResearchGate: https://www.researchgate.net/profile/Leland-Gee?ev=hdr_xprf

Professional

WORK EXPERIENCE

- NIH Ruth L. Kirschstein National Research Service Award Postdoctoral Fellow - Stanford University
- Laboratory Supervisor / Software Engineer - Crocker Nuclear Laboratory, University of California, Davis
- Neurobiology Research Intern - Neurobiology, Physiology and Behavior Department, UC Davis, Davis, CA

PROFESSIONAL AFFILIATIONS AND ACTIVITIES

- Member, Biophysical Society (2013 - present)
- Member, American Chemical Society (2014 - present)
- Member, Coblentz Society (2014 - present)
- Member, Society for Applied Spectroscopy (2014 - present)
- Leader, XSIM – NERSC High Performance Computing Project – "Computational simulations of advanced X-ray spectroscopy on biological metallocofactors" (2017 - present)
- Textbook Proposal Reviewer, Elsevier (2018 - 2018)
- X-ray User Proposal Reviewer, SSRL, SLAC (2018 - present)
- Dissertation Committee Member, Dept. of Chemistry, University of California, Davis (2019 - 2019)
- Member, American Association for the Advancement of Science (2020 - present)

Publications

PUBLICATIONS

- **Macromolecular crystallography and biology at the Linac Coherent Light Source.** *Journal of synchrotron radiation*
  Mous, S., Hunter, M. S., Poitevin, F., Boutet, S., Gee, L. B.
  2025
- **Unraveling Metal-Ligand Bonding in an HNO-Evolving {FeNO}6 Complex with a Combined X-ray Spectroscopic Approach.** *Journal of the American Chemical Society*
  Gee, L. B., Lim, J., Kroll, T., Sokaras, D., Alonso-Mori, R., Lee, C.
  2023
- **XFEL serial crystallography reveals the room temperature structure of methyl-coenzyme M reductase.** *Journal of inorganic biochemistry*
  Ohmer, C. J., Dasgupta, M., Patwardhan, A., Bogacz, I., Kaminsky, C., Doyle, M. D., Chen, P. Y., Keable, S. M., Makita, H., Simon, P. S., Massad, R., Fransson, T., Chatterjee, et al
  2022; 230: 111768
- **Carbon monoxide binding to alpha-R277H Mo-nitrogenase - Evidence for multiple pH-dependent species from IR-monitored photolysis.** *Journal of inorganic biochemistry*
  Gee, L. B., Scott, A. D., Dapper, C. H., Newton, W. E., Cramer, S. P.
  2022; 232: 111806
- **NRVS and DFT of MitoNEET: Understanding the Special Vibrational Structure of a [2Fe-2S] Cluster with (Cys)(3)(His)(1) Ligation** *BIOCHEMISTRY*
  Gee, L. B., Pelmenschikov, V., Mons, C., Mishra, N., Wang, H., Yoda, Y., Tamasaku, K., Golinelli-Cohen, M., Cramer, S. P.
  2021; 60 (31): 2419-2424

- **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

- **Valence-Dependent Electrical Conductivity in a 3D Tetrahydroxyquinone-Based Metal-Organic Framework.** *Journal of the American Chemical Society*
  Chen, G., Gee, L. B., Xu, W., Zhu, Y., Lezama-Pacheco, J. S., Huang, Z., Li, Z., Babicz, J. T., Choudhury, S., Chang, T., Reed, E., Solomon, E. I., Bao, et al
  2020

- **Vibrational characterization of a diiron bridging hydride complex - a model for hydrogen catalysis** *CHEMICAL SCIENCE*
  Gee, L. B., Pelmenschikov, V., Wang, H., Mishra, N., Liu, Y., Yoda, Y., Tamasaku, K., Chiang, M., Cramer, S. P.
  2020; 11 (21): 5487–93

- **Tuning the Geometric and Electronic Structure of Synthetic High-Valent Heme Iron(IV)-Oxo Models in the Presence of a Lewis Acid and Various Axial Ligands.** *Journal of the American Chemical Society*
  Ehudin, M. A., Gee, L. B., Sabuncu, S. n., Braun, A. n., Moënne-Loccoz, P. n., Hedman, B. n., Hodgson, K. O., Solomon, E. I., Karlin, K. D.
  2019; 141 (14): 5942–60

- **Synchrotron-based Nickel Mossbauer Spectroscopy** *INORGANIC CHEMISTRY*
  Gee, L. B., Lin, C., Jenney, F. E., Adams, M. W. W., Yoda, Y., Masuda, R., Saito, M., Kobayashi, Y., Tamasaku, K., Lerche, M., Seto, M., Riordan, C. G., Ploskonka, et al
  2016; 55 (14): 6866–72

- **X-ray Absorption Spectroscopy of Dilute Metalloenzymes at X-ray Free-Electron Lasers in a Shot-by-Shot Mode.** *The journal of physical chemistry letters*
  Bogacz, I., Szilagyi, E., Makita, H., Simon, P. S., Zhang, M., Doyle, M. D., Chatterjee, K., Kretzschmar, M., Chernev, P., Croy, N., Cheah, M. H., Dasgupta, M., Nangca, et al
  2025: 3778-3787

- **Experimental electronic structures of the FeIV=O bond in S=1 heme vs. nonheme sites: Effect of the porphyrin ligand.** *Proceedings of the National Academy of Sciences of the United States of America*
  Braun, A., Gee, L. B., Waters, M. D., Jose, A., Baker, M. L., Mara, M. W., Babicz, J. T., Ehudin, M. A., Quist, D. A., Zhou, A., Kroll, T., Titus, C. J., Lee, et al
  2025; 122 (8): e2420205122

- **Excited State Covalency, Dynamics, and Photochemistry of Square Planar Ni-Thiolate Complexes Revealed by Ultrafast X-ray Absorption.** *Journal of the American Chemical Society*
  Lim, H., Yang, X., Larsen, C. B., Ledbetter, K., Zoric, M. R., Raj, S. L., Kumar, G., Powers-Riggs, N., Hoffmann, M. C., Chollet, M., Gee, L. B., van Driel, T. B., Alonso-Mori, et al
  2025

- **Experimental Definition of the S = 1 π vs S = 2 σ Reactivity and S = 2 Character in the Ground State of an S = 1 FeIVO Complex.** *Journal of the American Chemical Society*
  Braun, A., Gee, L. B., Waters, M. D., Baker, M. L., Mara, M. W., Zhou, A., Kroll, T., Nordlund, D., Sokaras, D., Hedman, B., Hodgson, K. O., Que, L., Solomon, et al
  2024

- **New insights into the function and molecular mechanisms of Ferredoxin-NADP+ reductase from Brucella ovis.** *Archives of biochemistry and biophysics*
  Moreno, A., Quereda-Moraleda, I., Lozano-Vallhonrat, C., Buñuel-Escudero, M., Botha, S., Kupitz, C., Lisova, S., Sierra, R., Mariani, V., Schleissner, P., Gee, L. B., Dörner, K., Schmidt, et al
  2024; 762: 110204

- **Strain-affected ferroelastic domain walls in RbMnFe charge-transfer materials undergoing collective Jahn-Teller distortion.** *RSC advances*
  Herve, M., Akagi, S., Guerin, L., Gee, L. B., Ribson, R. D., Chollet, M., Cammarata, M., Nagashima, S., Ohkoshi, S., Tokoro, H., Collet, E.
  2024; 14 (47): 35081-35089

- **Time-Resolved X-ray Emission Spectroscopy and Synthetic High-Spin Model Complexes Resolve Ambiguities in Excited-State Assignments of Transition-Metal Chromophores: A Case Study of Fe-Amido Complexes.** *Journal of the American Chemical Society*

Reinhard, M. E., Sidhu, B. K., Lozada, I. B., Powers-Riggs, N., Ortiz, R. J., Lim, H., Nickel, R., Lierop, J. v., Alonso-Mori, R., Chollet, M., Gee, L. B., Kramer, P. L., Kroll, et al

2024

- **Temperature-dependent iron motion in extremophile rubredoxins - no need for 'corresponding states'.** *Scientific reports*

  Jenney, F. E., Wang, H., George, S. J., Xiong, J., Guo, Y., Gee, L. B., Marizcurrena, J. J., Castro-Sowinski, S., Staskiewicz, A., Yoda, Y., Hu, M. Y., Tamasaku, K., Nagasawa, et al

  2024; 14 (1): 12197

- **The Liquid Jet Endstation for Hard X-ray Scattering and Spectroscopy at the Linac Coherent Light Source.** *Molecules (Basel, Switzerland)*

  Antolini, C., Sosa Alfaro, V., Reinhard, M., Chatterjee, G., Ribson, R., Sokaras, D., Gee, L., Sato, T., Kramer, P. L., Raj, S. L., Hayes, B., Schleissner, P., Garcia-Esparza, et al

  2024; 29 (10)

- **An S = 1 Iron(IV) Intermediate Revealed in a Non-Heme Iron Enzyme-Catalyzed Oxidative C-S Bond Formation.** *Angewandte Chemie (International ed. in English)*

  Paris, J. C., Hu, S., Wen, A., Weitz, A. C., Cheng, R., Gee, L. B., Tang, Y., Kim, H., Vegas, A., Chang, W., Elliott, S. J., Liu, P., Guo, et al

  2023: e202309362

- **X-ray Spectroscopic Study of the Electronic Structure of a Trigonal High-Spin Fe(IV)═O Complex Modeling Non-Heme Enzyme Intermediates and Their Reactivity.** *Journal of the American Chemical Society*

  Braun, A., Gee, L. B., Mara, M. W., Hill, E. A., Kroll, T., Nordlund, D., Sokaras, D., Glatzel, P., Hedman, B., Hodgson, K. O., Borovik, A. S., Baker, M. L., Solomon, et al

  2023

- **Structural evidence for intermediates during O-2 formation in photosystem II** *NATURE*

  Bhowmick, A., Hussein, R., Bogacz, I., Simon, P. S., Ibrahim, M., Chatterjee, R., Doyle, M. D., Cheah, M., Fransson, T., Chernev, P., Kim, I., Makita, H., Dasgupta, et al

  2023: 629-636

- **Room temperature X-ray absorption spectroscopy of metalloenzymes with drop-on-demand sample delivery at XFELs** *PURE AND APPLIED CHEMISTRY*

  Bogacz, I., Makita, H., Simon, P. S. S., Zhang, M., Doyle, M. D. D., Chatterjee, R., Fransson, T., Weninger, C., Fuller, F., Gee, L., Sato, T., Seaberg, M., Alonso-Mori, et al

  2023

- **Investigation of the Structure of Atomically Dispersed NiNx Sites in Ni and N-Doped Carbon Electrocatalysts by 61Ni Mossbauer Spectroscopy and Simulations.** *Journal of the American Chemical Society*

  Koshy, D. M., Hossain, M. D., Masuda, R., Yoda, Y., Gee, L. B., Abiose, K., Gong, H., Davis, R., Seto, M., Gallo, A., Hahn, C., Bajdich, M., Bao, et al

  2022

- **Nitrogenase Chemistry at 10 Kelvin─Phototautomerization and Recombination of CO-Inhibited alpha-H195Q Enzyme.** *Inorganic chemistry*

  Gee, L. B., Myers, W. K., Nack-Lehman, P. A., Scott, A. D., Yan, L., George, S. J., Dong, W., Dapper, C. H., Newton, W. E., Cramer, S. P.

  2022; 61 (30): 11509-11513

- **Millisecond timescale reactions observed via X-ray spectroscopy in a 3D microfabricated fused silica mixer. Corrigendum.** *Journal of synchrotron radiation*

  Huyke, D. A., Ramachandran, A., Ramirez-Neri, O., Guerrero-Cruz, J. A., Gee, L. B., Braun, A., Sokaras, D., Garcia-Estrada, B., Solomon, E. I., Hedman, B., Delgado-Jaime, M. U., DePonte, D. P., Kroll, et al

  2022; 29 (Pt 3): 930

- **Nuclear Resonance Vibrational Spectroscopy: A Modern Tool to Pinpoint Site-Specific Cooperative Processes** *CRYSTALS*

  Wang, H., Braun, A., Cramer, S. P., Gee, L. B., Yoda, Y.

  2021; 11 (8)

- **Millisecond timescale reactions observed via X-ray spectroscopy in a 3D microfabricated fused silica mixer.** *Journal of synchrotron radiation*

  Huyke, D. A., Ramachandran, A., Ramirez-Neri, O., Guerrero-Cruz, J. A., Gee, L. B., Braun, A., Sokaras, D., Garcia-Estrada, B., Solomon, E. I., Hedman, B., Delgado-Jaime, M. U., DePonte, D. P., Kroll, et al

  2021; 28 (Pt 4): 1100-1113

- **Direct coordination of pterin to FeII enables neurotransmitter biosynthesis in the pterin-dependent hydroxylases.** *Proceedings of the National Academy of Sciences of the United States of America*

Iyer, S. R., Tidemand, K. D., Babicz, J. T., Jacobs, A. B., Gee, L. B., Haahr, L. T., Yoda, Y., Kurokuzu, M., Kitao, S., Saito, M., Seto, M., Christensen, H. E., Peters, et al

2021; 118 (15)

- **Effect of 3d/4p Mixing on 1s2p Resonant Inelastic X-ray Scattering: Electronic Structure of Oxo-Bridged Iron Dimers.** *Journal of the American Chemical Society*

  Kroll, T., Baker, M. L., Wilson, S. A., Lundberg, M., Juhin, A., Arrio, M., Yan, J. J., Gee, L. B., Braun, A., Weng, T., Sokaras, D., Hedman, B., Hodgson, et al

  2021

- **Nuclear Resonance Vibrational Spectroscopic Definition of the Fe(IV)2 Intermediate Q in Methane Monooxygenase and Its Reactivity.** *Journal of the American Chemical Society*

  Jacobs, A. B., Banerjee, R., Deweese, D. E., Braun, A., Babicz, J. T., Gee, L. B., Sutherlin, K. D., Böttger, L. H., Yoda, Y., Saito, M., Kitao, S., Kobayashi, Y., Seto, et al

  2021

- **Vibrational Perturbation of the [FeFe] Hydrogenase H-Cluster Revealed by 13C2H-ADT Labeling.** *Journal of the American Chemical Society*

  Pelmenschikov, V., Birrell, J. A., Gee, L. B., Richers, C. P., Reijerse, E. J., Wang, H., Arragain, S., Mishra, N., Yoda, Y., Matsuura, H., Li, L., Tamasaku, K., Rauchfuss, et al

  2021

- **High-Frequency Fe-H and Fe-H2 Modes in a trans-Fe(eta2-H2)(H) Complex: A Speed Record for Nuclear Resonance Vibrational Spectroscopy.** *Inorganic chemistry*

  Chiang, M., Pelmenschikov, V., Gee, L. B., Liu, Y., Hsieh, C., Wang, H., Yoda, Y., Matsuura, H., Li, L., Cramer, S. P.

  2020

- **Single-ion magnetism in the extended solid-state: insights from X-ray absorption and emission spectroscopy** *CHEMICAL SCIENCE*

  Huzan, M. S., Fix, M., Aramini, M., Bencok, P., Mosselmans, J. W., Hayama, S., Breitner, F. A., Gee, L. B., Titus, C. J., Arrio, M., Jesche, A., Baker, M. L.

  2020; 11 (43): 11801–10

- **Single-ion magnetism in the extended solid-state: insights from X-ray absorption and emission spectroscopy.** *Chemical science*

  Huzan, M. S., Fix, M., Aramini, M., Bencok, P., Mosselmans, J. F., Hayama, S., Breitner, F. A., Gee, L. B., Titus, C. J., Arrio, M. A., Jesche, A., Baker, M. L.

  2020; 11 (43): 11801-11810

- **Vibrational characterization of a diiron bridging hydride complex - a model for hydrogen catalysis.** *Chemical science*

  Gee, L. B., Pelmenschikov, V., Wang, H., Mishra, N., Liu, Y. C., Yoda, Y., Tamasaku, K., Chiang, M. H., Cramer, S. P.

  2020; 11 (21): 5487-5493

- **High-Frequency Fe-H Vibrations in a Bridging Hydride Complex Characterized by NRVS and DFT** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*

  Pelmenschikov, V., Gee, L. B., Wang, H., MacLeod, K., McWilliams, S. F., Skubi, K. L., Cramer, S. P., Holland, P. L.

  2018; 57 (30): 9367–71

- **Sterically Stabilized Terminal Hydride of a Diiron Dithiolate** *INORGANIC CHEMISTRY*

  Carlson, M. R., Gray, D. L., Richers, C. P., Wang, W., Zhao, P., Rauchfuss, T. B., Pelmenschikov, V., Pham, C. C., Gee, L. B., Wang, H., Cramer, S. P.

  2018; 57 (4): 1988–2001

- **NRVS for Fe in Biology: Experiment and Basic Interpretation.** *Methods in enzymology*

  Gee, L. B., Wang, H., Cramer, S. P.

  2018; 599: 409–25

- **Direct Observation of an Iron-Bound Terminal Hydride in [FeFe]-Hydrogenase by Nuclear Resonance Vibrational Spectroscopy** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

  Reijerse, E. J., Pham, C. C., Pelmenschikov, V., Gilbert-Wilson, R., Adamska-Venkatesh, A., Siebel, J. F., Gee, L. B., Yoda, Y., Tamasaku, K., Lubitz, W., Rauchfuss, T. B., Cramer, S. P.

  2017; 139 (12): 4306–9

- **Is trehalose an effective quenching agent of Azotobacter vinelandii Mo-nitrogenase turnover?** *INORGANICA CHIMICA ACTA*

  Gee, L. B., Scott, A. D., Dapper, C. H., Newton, W. E., Cramer, S. P.

2016; 453: 74–77

- **Characterization of the [3Fe-4S](0/1+) cluster from the D14C variant of Pyrococcus furiosus ferredoxin via combined NRVS and DFT analyses** *DALTON TRANSACTIONS*
  Lauterbach, L., Gee, L. B., Pelmenschikov, V., Jenney, F. E., Kamali, S., Yoda, Y., Adams, M. W. W., Cramer, S. P.
  2016; 45 (17): 7215–19
- **Low frequency dynamics of the nitrogenase MoFe protein via femtosecond pump probe spectroscopy - Observation of a candidate promoting vibration** *JOURNAL OF INORGANIC BIOCHEMISTRY*
  Maiuri, M., Delfino, I., Cerullo, G., Manzoni, C., Pelmenschikov, V., Guo, Y., Wang, H., Gee, L. B., Dapper, C. H., Newton, W. E., Cramer, S. P.
  2015; 153: 128–35
- **Hydride bridge in [NiFe]-hydrogenase observed by nuclear resonance vibrational spectroscopy** *NATURE COMMUNICATIONS*
  Ogata, H., Kraemer, T., Wang, H., Schilter, D., Pelmenschikov, V., van Gastel, M., Neese, F., Rauchfuss, T. B., Gee, L. B., Scott, A. D., Yoda, Y., Tanaka, Y., Lubitz, et al
  2015; 6: 7890
- **Docking and Migration of Carbon Monoxide in Nitrogenase: The Case for Gated Pockets from Infrared Spectroscopy and Molecular Dynamics** *BIOCHEMISTRY*
  Gee, L. B., Leontyev, I., Stuchebrukhov, A., Scott, A. D., Pelmenschikov, V., Cramer, S. P.
  2015; 54 (21): 3314–19
- **Nuclear resonance vibrational spectroscopy reveals the FeS cluster composition and active site vibrational properties of an O-2-tolerant NAD(+)-reducing [NiFe] hydrogenase** *CHEMICAL SCIENCE*
  Lauterbach, L., Wang, H., Horch, M., Gee, L. B., Yoda, Y., Tanaka, Y., Zebger, I., Lenz, O., Cramer, S. P.
  2015; 6 (2): 1055–60
- **Synthesis and vibrational spectroscopy of Fe-57-labeled models of [NiFe] hydrogenase: first direct observation of a nickel-iron interaction** *CHEMICAL COMMUNICATIONS*
  Schilter, D., Pelmenschikov, V., Wang, H., Meier, F., Gee, L. B., Yoda, Y., Kaupp, M., Rauchfuss, T. B., Cramer, S. P.
  2014; 50 (88): 13469–72
- **In Silico Dynamics of Carbon Monoxide in the Active Site Pocket of Nitrogenase**
  Gee, L. B., Leontyev, I., Cramer, S. P.
  CELL PRESS.2014: 608A
- **Differences in peripheral endocannabinoid modulation of scratching behavior in facial vs. spinally-innervated skin** *NEUROPHARMACOLOGY*
  Spradley, J., Davoodi, A., Gee, L., Carstens, M., Carstens, E.
  2012; 63 (4): 743–49

PRESENTATIONS

- MFX-HE: Opportunities for High-Throughput Multimodal Structural Studies and Their Computational Challenges - SLAC User Workshop (9/27/2024)
- Linking Theory and X-ray Spectroscopy of Metallocofactors and Inorganic Systems - SLAC User Workshop (9/22/2024)
- Plenary Session - Synergy at SLAC I/II: Cooperative Science Utilizing the LCLS and SSRL - SLAC User Workshop (9/28/2022)
- Developments of X-ray Spectroscopy at the LCLS Towards Applications to Biomedical Research - BioXFEL (2/8/2022 - 2/10/2022)
- Applications of Soft X-ray Spectroscopy to Biological Systems - Soft X-ray RIXS Workshop (2/3/2020)
- A Gated Substrate Channel In Nitrogenase Revealed Through a Combined IR and Molecular Dynamics Study - 19th International Congress on Nitrogen Fixation