

LELAND B. GEE

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EDUCATION

University of California, Davis
Davis, California

Ph.D. Biophysics

Dissertation: "X-ray and Infrared Spectroscopic Investigations of Nitrogenase and Hydrogenase"

September 24, 2012 – December 9, 2016

University of California, Davis
Davis, California

B.S. Biochemistry and Molecular Biology

B.A. Economics

September 20, 2007 – June 9, 2011

PROFESSIONAL CAREER

Linac Coherent Light Source, SLAC National Accelerator Facility, Menlo Park, CA
Project Scientist

May 2021 – Current

Chemistry Department, Stanford University, Stanford, CA
NIH Ruth L. Kirschstein National Research Service Award Postdoctoral Fellow

November 2016 – May 2021

Chemistry Department, UC Davis, Davis, CA
Graduate Student Researcher

September 2012 – November 2016

Crocker Nuclear Laboratory, UC Davis, Davis, CA
Programmer/Laboratory Supervisor

March 2011 – October 2012

Neurobiology, Physiology and Behavior Department, UC Davis, Davis, CA
Student Assistant

February 2010 – March 2011

SCIENTIFIC COMMUNITY ROLES

Textbook Proposal Reviewer – 2018 – Elsevier

X-ray User Proposal Reviewer – 2018-2021 – SLAC

Graduate Student Dissertation Committee Member – 2019 – UC Davis Chemistry Department

Independent Scientific Consultant – 2020-2021 – SETI Institute

Leader of XSIM – NERSC High Performance Computing Project – 2017-2021:

"Computational simulations of advanced X-ray spectroscopy on biological metallocofactors"

Developer of spectra.tools website to analyze spectroscopic data – 2015-2021 – facilitating 20 publications globally

MEMBERSHIPS

American Chemical Society (Since 2014)

Biophysical Society (Since 2013)

Society for Applied Spectroscopy (Since 2014)

Coblentz Society (Since 2014)

American Association for the Advancement of Science (Since 2020)

AWARDS

UC Davis and Humanities Graduate Student Research Award (2015)

Biophysical Society Educational Committee Travel Award (2016)

NIH Ruth L. Kirschstein National Research Service Award (2017-2021)

PRESENTATIONS

Applications of Soft X-ray Spectroscopy to Biological Systems

Invited Speaker at the **2020** Soft X-ray RIXS Workshop at SLAC. Menlo Park, CA

Application of Synchrotron-based Nickel Mössbauer Spectroscopy on Enzymes

Poster presented at the **2016** Metallocofactors Gordon Research Conference. Easton, MA

A Gated Substrate Channel In Nitrogenase Revealed Through a Combined IR and Molecular Dynamics Study

Education Committee Travel Award Winner at the **2016** Biophysical Society Conference. Los Angeles, CA

A Gated Substrate Channel In Nitrogenase Revealed Through a Combined IR and Molecular Dynamics Study

Invited Speaker at the **2015** 19th International Congress on Nitrogen Fixation. Pacific Grove, CA

Chemistry Below 10K? EPR and IR investigation of H195Q CO-bound Nitrogenase

Poster Presented at the **2015** 19th International Congress on Nitrogen Fixation. Pacific Grove, CA

Nuclear resonant vibrational spectroscopy in studying extremely weak features in hydrogenases and nitrogenases

Poster presented at the **2014** National ACS Conference. San Francisco, CA

In Silico Dynamics of Carbon Monoxide in the Active Site Pocket of Nitrogenase

Poster presented at the **2014** Biophysical Society Conference. San Francisco, CA

- 25. Leland B. Gee, Vladimir Pelmentschikov, Cécile Mons, Nakul Mishra, Hongxin Wang, Yoshitaka Yoda, Kenji Tamasaku, Marie-Pierre Golinelli-Cohen, and Stephen P. Cramer**
NRVS and DFT of MitoNEET – Understanding the Special Vibrational Structure of a [2Fe-2S] Cluster with (Cys)₃(His)₁ Ligation. *Inorganic Chemistry*. **2021**. In Revision.
- 24. Vladimir Pelmentschikov, James A. Birrell, Leland B. Gee, Casseday P. Richers, Edward J. Reijerse, Hongxin Wang, Simon Arragain, Nakul Mishra, Yoshitaka Yoda, Hiroaki Matsuura, Lei Li, Kenji Tamasaku, Thomas B. Rauchfuss, Wolfgang Lubitz, Stephen P. Cramer**
Vibrational Perturbation of the [FeFe] Hydrogenase H-cluster Revealed by a ¹³C²H-ADT Labeling. *Journal of the American Chemical Society*. **2021**. In Press.
- 23. Diego A. Huyke, Ashwin Ramachandran, Oscar Ramirez-Neri, Jose A. Guerrero-Cruz, Leland B. Gee, Augustin Braun, Dimosthenis Sokaras, Brenda Garcia-Estrada, Edward I. Solomon, Britt Hedman, Mario U. Delgado-Jaime, Daniel P. DePonte, Thomas Kroll, Juan G. Santiago**
Three dimensional hydrodynamic focusing and mixing in a monolithic fused silica microfluidic device. *Journal Of Synchrotron Radiation*. **2021**. In Press.
- 22. Thomas Kroll, Michael L. Baker, Samuel A. Wilson, Marcus Lundberg, Amélie Juhin, Marie-Anne Arrio, James J. Yan, Leland B. Gee, Tsu-Chien Weng, Dimosthenis Sokaras, Britt Hedman, Keith O. Hodgson, Edward I. Solomon.**
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*. **2021**. 143 (12), 4569-4584. DOI: 10.1021/jacs.0c11193
- 21. Shyam R. Iyer, Kasper D. Tidemand, Jeffrey T. Babicz Jr., Ariel B. Jacobs, Leland B. Gee, Lærke T Haahr, Yoshitaka Yoda, Masayuki Kurokuzu, Shinji Kitao, Makina Saito, Makoto Seto, Hans Christensen, Günther H. J. Peters, Edward I. Solomon.**
Direct Coordination of Pterin to Fe^{II} Enables Neurotransmitter Biosynthesis in the Pterin-dependent Hydroxylases. *PNAS*. **2021**. 118 (15), DOI: 10.1073/pnas.2022379118
- 20. Marco E. Reinhard, Michael W. Mara, Thomas Kroll, Hyeongtaek Lim, Ryan G. Hadt, Roberto Alonso-Mori, Matthieu Chollet, James M. Glowacki, Silke Nelson, Dimosthenis Sokaras, Kristjan Kunnus, Tim Brandt van Driel, Robert W. Hartsock, Kasper S. Kjaer, Clemens Weninger, Elisa Biasin, Leland B. Gee, Keith O. Hodgson, Britt Hedman, Uwe Bergmann, Edward I. Solomon, Kelly J. Gaffney**
Short-lived metal-centered excited state initiates iron-methionine photodissociation in ferrous cytochrome c. *Nature Communications*. **2021**. *Nature Communications*. Feb 17; 12:1086. DOI: 10.1038/s41467-021-21423-w
- 19. Ming-Hsi Chiang & Vladimir Pelmentschikov & Leland B. Gee, Yu-Chiao Liu, Hongxin Wang, Yoshitaka Yoda, Hiroaki Matsuura, Lei Li, Stephen P. Cramer**
The detailed H-Fe-H₂ vibrational structure of a molecular dihydrogen complex – A New Speed Record for Nuclear Resonance Vibrational Spectroscopy. *Inorg. Chem*. **2021**, 60, 2, 555–559. DOI:10.1021/acs.inorgchem.0c03006
- 18. Gan Chen, Leland B. Gee, Wenqian Xu, Yanbing Zhu, Juan S. Lezama-Pacheco, Zhehao Huang, Zongqi Li, Snehashis Choudhury, Ting-Hsiang Chang, Evan Reed, Edward I. Solomon, Zhenan Bao**
Valence Dependent Electrical Conductivity in a 3D Tetrahydroxyquinone Based Metal–Organic Framework. *Journal of the American Chemical Society*. **2020**, 142, 51, 21243–21248 DOI:10.1021/jacs.0c09379
- 17. Myron S. Huzan, Manuel Fix, Matteo Aramini, Peter Bencok, J. Frederick W. Mosselmans, Shusaku Hayama, Franziska A. Breitner, Leland B. Gee, Charles J. Titus, Marie-Anne Arrio, Anton Jesche, Michael L. Baker.**
Single-ion magnetism in the extended solid-state: insights from X-ray absorption and emission spectroscopy. *Chemical Science*, **2020**, 11, 11801-11810. DOI:10.1039/D0SC03787G
- 16. Leland B. Gee, Hongxin Wang, Stephen P. Cramer**
Nuclear Resonance Vibrational Spectroscopy. In *Bioorganometallic Chemistry*, 1st ed.; Wolfgang Weigand and Ulf-Peter Apfel, Eds. De Gruyter: Berlin, Germany. **2020**; pp. 353-394. DOI:10.1515/9783110496574-009
- 15. Leland B. Gee, Vladimir. Pelmentschikov, Hongxin Wang, Nakul Mishra, Yu-Chiao Liu, Yoshitaka Yoda, Ming Hsi Chiang & Stephen P. Cramer**
Vibrational and electronic characterization of a diiron bridging hydride complex – a model for hydrogen catalysis. *Chemical Science*, **2020**, 11, 5487-5493. DOI:10.1039/d0sc01290d
- 14. Melanie A. Ehudin & Leland B. Gee, Sinan Sabuncu, Augustin Braun, Pierre Moënné-Loccoz, Britt Hedman, Keith O. Hodgson, Edward I. Solomon & Kenneth D. Karlin**
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*, **2019**, 141, 5942-5960. DOI:10.1021/jacs.9b00795
- 13. Vladimir Pelmentschikov, Leland B. Gee, Hongxin Wang, Cory K. MacLeod, Sean F. McWilliams, Kazimer L. Skubi, Stephen P. Cramer, Patrick L. Holland**
High-Frequency Fe–H Vibrations in a Bridging Hydride Complex Characterized by NRVS and DFT. *Angew. Chem., Int. Ed.* **2018**, 130 (30), 9511-9515. DOI:10.1002/ange.201804601

12. Michaela R. Carlson, Danielle L. Gray, Casseday P. Richers, Wenguang Wang, Pei-Hua Zhao, Thomas B. Rauchfuss, Vladimir Pelmentschikov, Cindy C. Pham, Leland B. Gee, Hongxin Wang, Stephen P. Cramer
Sterically Stabilized Terminal Hydride of a Diiron Dithiolate. *Inorg Chem* **2018**, 57 (4), 1988-2001.
DOI:10.1021/acs.inorgchem.7b02903

11. Leland B. Gee, Hongxin Wang, Stephen P. Cramer
NRVS For Fe in Biology: Experiment and Basic Interpretation. In *Methods in Enzymology: Fe-S Cluster Enzymes*, 1st ed.; Sheila S. David, Ed. Academic Press: Cambridge, MA, **2018**; Vol. 599, pp 409-426. DOI:10.1016/bs.mie.2017.11.002

10. Edward J. Reijerse, Cindy C. Pham, Vladimir Pelmentschikov, Ryan Gilbert-Wilson, Agnieszka Adamska-Venkatesh, Judith F. Siebel, Leland B. Gee, Yoshitaka Yoda, Kenji Tamasaku, Wolfgang Lubitz, Thomas B. Rauchfuss, Stephen P. Cramer
Direct Observation of an Iron-Bound Terminal Hydride in [FeFe]-Hydrogenase by Nuclear Resonance Vibrational Spectroscopy. *J Am Chem Soc.* **2017**, 139, 4306-4309 DOI: 10.1021/jacs.7b00686

9. Leland B. Gee, Aubrey D. Scott, Christie H. Dapper, William E. Newton, Stephen P. Cramer
Is Trehalose an Effective Quenching Agent of Azotobacter vinelandii Mo-Nitrogenase Turnover?. *Inorganica Chimica Acta*. **453**. **2016**. DOI:10.1016/j.ica.2016.07.039

8. Leland B. Gee, Chun-Yi Lin, Francis E. Jenney Jr., Michael W.W. Adams, Yoshitaka Yoda, Ryo Masuda, Makina Saito, Yasuhiro Kobayashi, Kenji Tamasaku, Michael Lerche, Makoto Seto, Charles G. Riordan, Ann Ploskonka, Philip P. Power, Stephen P. Cramer, Lars Lauterbach
Synchrotron-based Nickel Mössbauer Spectroscopy. *Inorg. Chem.*, **2016**, 55 (14), pp 6866–6872.
DOI:10.1021/acs.inorgchem.5b03004

7. Lars Lauterbach, Leland B. Gee, Vladimir Pelmentschikov, Francis E. Jenney Jr., Saeed Kamali, Yoshitaka Yoda, Michael W. Adams, Stephen P. Cramer
Characterization of the [3Fe-4S]^{0/1+} cluster from the D14C variant of Pyrococcus furiosus ferredoxin via combined NRVS and DFT analyses. *Dalton Trans.*, **2016**, 45, 7215-7219. DOI:10.1039/C5DT04760A

6. Margherita Maiuri, Ines Delfino, Giulio Cerullo, Cristian Manzoni, Vladimir Pelmentschikov, Yisong Guo, Hongxin Wang, Leland B. Gee, Christie H. Dapper, William E. Newton, Stephen P. Cramer
Low Frequency Dynamics of the Nitrogenase MoFe Protein via Femtosecond Pump Probe Spectroscopy – Observation of a Candidate Promoting Vibration. *J. Inorganic Biochemistry* **2015**. Dec; 153:128-35. DOI:10.1016/j.jinorgbio.2015.07.005

5. Hideaki Ogata, Tobias Kramer, Hongxin Wang, David Schilter, Vladimir Pelmentschikov, Maurice van Gastel, Frank Neese, Thomas Rauchfuss, Leland B. Gee, Aubrey Scott, Yoshitaka Yoda, Yoshihito Tanaka, Wolfgang Lubitz, Stephen Cramer
Hydride bridge in NiFe-hydrogenase observed by nuclear resonance vibrational spectroscopy. *Nature Communications*. **2015**. Aug 10;6:7890. DOI:10.1038/ncomms8890

4. Leland B. Gee, Igor Leontyev, Alexei Stuchebrukhov, Aubrey Scott, Vladimir Pelmentschikov, Stephen P. Cramer
Docking and Migration of Carbon Monoxide in Nitrogenase – The Case for Gated Pockets from IR Spectroscopy and Molecular Dynamics. *Biochemistry*. **2015**. 54(21), 3314-3319. DOI:10.1021/acs.biochem.5b00216

3. Lars Lauterbach, Hongxin Wang, Marius Horch, Leland B. Gee, Yoshitaka Yoda, Yoshihito Tanaka, Ingo Zebger, Oliver Lenz, Stephen P. Cramer
Nuclear resonance vibrational spectroscopy reveals the FeS cluster composition and active site vibrational properties of an O₂-tolerant NAD⁺-reducing [NiFe] hydrogenase. *Chemical Science* **2015**, 6, 1055-1060. DOI:10.1039/C4SC02982H

2. David Schilter, Hongxin Wang, Vladimir Pelmentschikov, Leland B. Gee, Yoshitaka Yoda, Stephen P. Cramer
Synthesis and Vibrational Spectroscopy of ⁵⁷Fe-Labeled Models of [NiFe] Hydrogenase: First Direct Observation of a Nickel-Iron Interaction. *Chem. Commun.* **2014**, 50, 13469-13472. DOI:10.1039/C4CC04572F

1. Jessica M. Spradley, Auva Davoodi, Leland B. Gee, Mirela. I. Carstens, Earl Carstens.
Differences in peripheral endocannabinoid modulation of scratching behavior in facial vs. spinally-innervated skin. *Neuropharmacology*. **2012**. 63(4), 743–9. DOI:10.1016/j.neuropharm.2012.05.032