

# Stanford

---

## Lei Liu

Masters Student in Management Science and Engineering, admitted Autumn 2020

### Publications

---

#### PUBLICATIONS

- **Nuclear Resonance Vibrational Spectroscopy Definition of O<sub>2</sub> Intermediates in an Extradiol Dioxygenase: Correlation to Crystallography and Reactivity**. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*  
Sutherlin, K. D., Wasada-Tsutsui, Y., Mbughuni, M. M., Rogers, M. S., Park, K., Liu, L., Kwak, Y., Srnec, M., Bottger, L. H., Frenette, M., Yoda, Y., Kobayashi, Y., Kurokuzu, et al  
2018; 140 (48): 16495–513
- **Nuclear Resonance Vibrational Spectroscopy Definition of O<sub>2</sub> Intermediates in an Extradiol Dioxygenase: Correlation to Crystallography and Reactivity**. *Journal of the American Chemical Society*  
Sutherlin, K. D., Wasada-Tsutsui, Y., Mbughuni, M. M., Rogers, M. S., Park, K., Liu, L. V., Kwak, Y., Srnec, M., Bottger, L. H., Frenette, M., Yoda, Y., Kobayashi, Y., Kurokuzu, et al  
2018
- **NRVS Studies of the Peroxide Shunt Intermediate in a Rieske Dioxygenase and Its Relation to the Native Fe-II O<sub>2</sub> Reaction** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*  
Sutherlin, K. D., Rivard, B. S., Bottger, L. H., Liu, L. V., Rogers, M. S., Srnec, M., Park, K., Yoda, Y., Kitao, S., Kobayashi, Y., Saito, M., Seto, M., Hu, et al  
2018; 140 (16): 5544–59
- **Peroxide Activation for Electrophilic Reactivity by the Binuclear Non-heme Iron Enzyme AurF**. *Journal of the American Chemical Society*  
Park, K., Li, N., Kwak, Y., Srnec, M., Bell, C. B., Liu, L. V., Wong, S. D., Yoda, Y., Kitao, S., Seto, M., Hu, M., Zhao, J., Krebs, et al  
2017; 139 (20): 7062-7070
- **Nuclear Resonance Vibrational Spectroscopic Definition of Peroxy Intermediates in Nonheme Iron Sites**. *Journal of the American Chemical Society*  
Sutherlin, K. D., Liu, L. V., Lee, Y., Kwak, Y., Yoda, Y., Saito, M., Kurokuzu, M., Kobayashi, Y., Seto, M., Que, L., Nam, W., Solomon, E. I.  
2016; 138 (43): 14294-14302
- **Geometric and electronic structure of the Mn(IV)Fe(III) cofactor in class Ic ribonucleotide reductase: correlation to the class Ia binuclear non-heme iron enzyme**. *Journal of the American Chemical Society*  
Kwak, Y., Jiang, W., Dassama, L. M., Park, K., Bell, C. B., Liu, L. V., Wong, S. D., Saito, M., Kobayashi, Y., Kitao, S., Seto, M., Yoda, Y., Alp, et al  
2013; 135 (46): 17573-17584
- **Geometric and Electronic Structure of the Mn(IV)Fe(III) Cofactor in Class Ic Ribonucleotide Reductase: Correlation to the Class Ia Binuclear Non-Heme Iron Enzyme**. *Journal of the American Chemical Society*  
Kwak, Y., Jiang, W., Dassama, L. M., Park, K., Bell, C. B., Liu, L. V., Wong, S. D., Saito, M., Kobayashi, Y., Kitao, S., Seto, M., Yoda, Y., Alp, et al  
2013; 135 (46): 17573-17584
- **Geometric and Electronic Structure Contributions to Function in Non-heme Iron Enzymes** *ACCOUNTS OF CHEMICAL RESEARCH*  
Solomon, E. I., Light, K. M., Liu, L. V., Srnec, M., Wong, S. D.  
2013; 46 (11): 2725-2739
- **Elucidation of the Fe(IV)=O intermediate in the catalytic cycle of the halogenase SyrB2**. *Nature*  
Wong, S. D., Srnec, M., Matthews, M. L., Liu, L. V., Kwak, Y., Park, K., Bell, C. B., Alp, E. E., Zhao, J., Yoda, Y., Kitao, S., Seto, M., Krebs, et al  
2013; 499 (7458): 320-323
- **Elucidation of the Fe(IV)=O intermediate in the catalytic cycle of the halogenase SyrB2** *NATURE*  
Wong, S. D., Srnec, M., Matthews, M. L., Liu, L. V., Kwak, Y., Park, K., Bell, C. B., Alp, E. E., Zhao, J., Yoda, Y., Kitao, S., Seto, M., Krebs, et al  
2013; 499 (7458): 320-?

- **Nuclear resonance vibrational spectroscopic and computational study of high-valent diiron complexes relevant to enzyme intermediates.** *Proceedings of the National Academy of Sciences of the United States of America*  
Park, K., Bell, C. B., Liu, L. V., Wang, D., Xue, G., Kwak, Y., Wong, S. D., Light, K. M., Zhao, J., Alp, E. E., Yoda, Y., Saito, M., Kobayashi, et al  
2013; 110 (16): 6275-6280
- **Nuclear resonance vibrational spectroscopic and computational study of high-valent diiron complexes relevant to enzyme intermediates** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*  
Park, K., Bell, C. B., Liu, L. V., Wang, D., Xue, G., Kwak, Y., Wong, S. D., Light, K. M., Zhao, J., Alp, E. E., Yoda, Y., Saito, M., Kobayashi, et al  
2013; 110 (16): 6269-6280
- **Comparison of High-Spin and Low-Spin Nonheme Fe-III-O<sub>2</sub>H Complexes in O-O Bond Homolysis and H-Atom Abstraction Reactivities** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*  
Liu, L. V., Hong, S., Cho, J., Nam, W., Solomon, E. I.  
2013; 135 (8): 3286-3299
- **Nuclear Resonance Vibrational Spectroscopy and DFT study of Peroxo-Bridged Biferric Complexes: Structural Insight into Peroxo Intermediates of Binuclear Non-heme Iron Enzymes** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*  
Park, K., Tsugawa, T., Furutachi, H., Kwak, Y., Liu, L. V., Wong, S. D., Yoda, Y., Kobayashi, Y., Saito, M., Kurokuzu, M., Seto, M., Suzuki, M., Solomon, et al  
2013; 52 (4): 1294-1298
- **Mononuclear nickel(II)-superoxo and nickel(III)-peroxo complexes bearing a common macrocyclic TMC ligand** *CHEMICAL SCIENCE*  
Cho, J., Kang, H. Y., Liu, L. V., Sarangi, R., Solomon, E. I., Nam, W.  
2013; 4 (4): 1502-1508
- **Structure and reactivity of a mononuclear non-haem iron(III)-peroxo complex** *NATURE*  
Cho, J., Jeon, S., Wilson, S. A., Liu, L. V., Kang, E. A., Braymer, J. J., Lim, M. H., Hedman, B., Hodgson, K. O., Valentine, J. S., Solomon, E. I., Nam, W.  
2011; 478 (7370): 502-505
- **Variable-temperature variable-field magnetic circular dichroism (VTVH MCD) and nuclear resonance vibrational spectroscopy (NRVS) studies on Fe-IV=O intermediates: Electronic and geometric structural insight into reactivity** *241st National Meeting and Exposition of the American-Chemical-Society (ACS)*  
Wong, S. D., Bell, C. B., Liu, L. V., Kwak, Y., England, J., Zhao, J., Que, L., Solomon, E. I.  
AMER CHEMICAL SOC.2011
- **S K-Edge X-Ray Absorption Spectroscopy and Density Functional Theory Studies of High and Low Spin {FeNO}(7) Thiolate Complexes: Exchange Stabilization of Electron Delocalization in {FeNO}(7) and {FeO<sub>2</sub>}(8)** *INORGANIC CHEMISTRY*  
Sun, N., Liu, L. V., Dey, A., Villar-Acevedo, G., Kovacs, J. A., Daresbourg, M. Y., Hodgson, K. O., Hedman, B., Solomon, E. I.  
2011; 50 (2): 427-436
- **Nuclear Resonance Vibrational Spectroscopy on the Fe-IV=O S=2 Non-Heme Site in TMG(3)tren: Experimentally Calibrated Insights into Reactivity** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*  
Wong, S. D., Bell, C. B., Liu, L. V., Kwak, Y., England, J., Alp, E. E., Zhao, J., Que, L., Solomon, E. I.  
2011; 50 (14): 3215-3218
- **Definition of the intermediates and mechanism of the anticancer drug bleomycin using nuclear resonance vibrational spectroscopy and related methods** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*  
Liu, L. V., Bell, C. B., Wong, S. D., Wilson, S. A., Kwak, Y., Chow, M. S., Zhao, J., Hodgson, K. O., Hedman, B., Solomon, E. I.  
2010; 107 (52): 22419-22424
- **S K-Edge X-Ray Absorption Spectroscopy and Density Functional Theory Studies of High and Low Spin {FeNO}(7) Thiolate Complexes: Exchange Stabilization of Electron Delocalization in {FeNO}(7) and {FeO(2)}(8).** *Inorganic chemistry*  
Sun, N., Liu, L. V., Dey, A., Villar-Acevedo, G., Kovacs, J. A., Daresbourg, M. Y., Hodgson, K. O., Hedman, B., Solomon, E. I.  
2010
- **Spectroscopic and DFT studies of activated bleomycin and its reactivity**  
Liu, L. V., Chow, M. S., Bell, C. B., Wong, S. D., Zhao, J., Solomon, E. I.  
AMER CHEMICAL SOC.2010
- **Theoretical studies on structures, C-13 NMR chemical shifts, aromaticity, and chemical reactivity of finite-length open-ended armchair single-walled carbon nanotubes** *NANOSCALE*  
Liu, L. V., Tian, W. Q., Chen, Y. K., Zhang, Y. A., Wang, Y. A.

2010; 2 (2): 254-261

● **Peroxo and oxo intermediates in mononuclear nonheme iron enzymes and related active sites** *CURRENT OPINION IN CHEMICAL BIOLOGY*

Solomon, E. I., Wong, S. D., Liu, L. V., Decker, A., Chow, M. S.  
2009; 13 (1): 99-113

● **Further insights into the mechanism of the reaction of activated bleomycin with DNA** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

Chow, M. S., Liu, L. V., Solomon, E. I.  
2008; 105 (36): 13241-13245

● **Ozonization at the vacancy defect site of the single-walled carbon nanotube** *JOURNAL OF PHYSICAL CHEMISTRY B*

Liu, L. V., Tian, W. Q., Wang, Y. A.  
2006; 110 (26): 13037-13044

● **Chemical reaction of nitric oxides with the 5-1DB defect of the single-walled carbon nanotube** *JOURNAL OF PHYSICAL CHEMISTRY B*

Liu, L. V., Tian, W. Q., Wang, Y. A.  
2006; 110 (5): 1999-2005

● **Electronic properties and reactivity of Pt-doped carbon nanotubes** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*

Tian, W. Q., Liu, L. V., Wang, Y. A.  
2006; 8 (30): 3528-3539