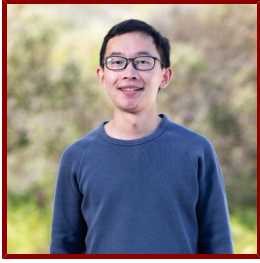


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Xiang Li

Associate Scientist, SLAC National Accelerator Laboratory

Bio

BIO

I am a scientist in the AMO Sciences Department and Data Systems Division at the LCLS. Investigating the ultrafast processes in atoms and molecules with charged-particle spectroscopy at x-ray free-electron lasers is the major theme of my research. It consists of three interconnected endeavors. One is to understand the material response to ultra-intense x-rays at the atomic level, and another is to exploit such x-rays as the probe for unraveling photo-induced molecular dynamics. And the third is to develop machine learning algorithms for solving some of the bottleneck problems in our field. I am involved in the design, assembly, and operation of experimental endstations at the AMO beamline of the LCLS, as well as the software development for AMO experiments performed at free-electron laser facilities.

EDUCATION AND CERTIFICATIONS

- Ph.D., Kansas State University , Physics (2019)
- B.S., South China Normal University/Kansas State University , Physics (2014)

LINKS

- Google Scholar: <https://scholar.google.com/citations?user=ugcdWMgAAAAJ&hl=en>
- GitHub: <https://github.com/xli025>
- LCLS AMO Sciences Department: <https://lcls.slac.stanford.edu/depts/amo>
- LCLS Data Systems Division: <https://lcls.slac.stanford.edu/depts/data-systems>

Publications

PUBLICATIONS

- **Generative modeling enables molecular structure retrieval from Coulomb explosion imaging.** *Nature communications*
Li, X., Jahnke, T., Boll, R., Han, J., Xu, M., Meyer, M., Piancastelli, M. N., Rolles, D., Rudenko, A., Trinter, F., Wolf, T. J., Thayer, J. B., Cryan, et al
2026
- **Attosecond X-Ray Core-Level Chronoscopy of Aromatic Molecules** *PHYSICAL REVIEW X*
Ji, J., Guo, Z., Driver, T., Trevisan, C. S., Cesar, D., Cheng, X., Duris, J., Franz, P. L., Glowina, J., Gong, X., Hammerland, D., Han, M., Heck, et al
2025; 15 (4)
- **Visualizing the Three-Dimensional Arrangement of Hydrogen Atoms in Organic Molecules by Coulomb Explosion Imaging.** *Journal of the American Chemical Society*
Green, A. E., Chen, K., Bhattacharyya, S., Allum, F., Usenko, S., Ashfold, M. N., Baumann, T. M., Borne, K. D., Brouard, M., Burt, M., Curchod, B. F., Erk, B., Forbes, et al
2025

- **Imaging collective quantum fluctuations of the structure of a complex molecule.** *Science (New York, N.Y.)*
Richard, B., Boll, R., Banerjee, S., Schäfer, J. M., Jurek, Z., Kastirke, G., Fehre, K., Schöffler, M. S., Anders, N., Baumann, T. M., Eckart, S., Erk, B., De Fanis, et al
2025; 389 (6760): 650-654
- **Imaging a light-induced molecular elimination reaction with an X-ray free-electron laser.** *Nature communications*
Li, X., Boll, R., Vindel-Zandbergen, P., González-Vázquez, J., Rivas, D. E., Bhattacharyya, S., Borne, K., Chen, K., De Fanis, A., Erk, B., Forbes, R., Green, A. E., Ilchen, et al
2025; 16 (1): 7006
- **The time-resolved atomic, molecular and optical science instrument at the Linac Coherent Light Source. Corrigendum.** *Journal of synchrotron radiation*
Walter, P., Osipov, T., Lin, M. F., Cryan, J., Driver, T., Kamalov, A., Marinelli, A., Robinson, J., Seaberg, M. H., Wolf, T. J., Aldrich, J., Brown, N., Champenois, et al
2025
- **Non-linear enhancement of ultrafast X-ray diffraction through transient resonances.** *Nature communications*
Kuschel, S., Ho, P. J., Al Haddad, A., Zimmermann, F. F., Flueckiger, L., Ware, M. R., Duris, J., MacArthur, J. P., Lutman, A., Lin, M. F., Li, X., Nakahara, K., Aldrich, et al
2025; 16 (1): 847
- **Probing Electronic Coherence between Core-Level Vacancies at Different Atomic Sites** *PHYSICAL REVIEW X*
Wang, J., Driver, T.
2025; 15: 011008
- **Design and performance of a magnetic bottle electron spectrometer for high-energy photoelectron spectroscopy.** *The Review of scientific instruments*
Borne, K., O'Neal, J. T., Wang, J., Isele, E., Obaid, R., Berrah, N., Cheng, X., Bucksbaum, P. H., James, J., Kamalov, A., Larsen, K. A., Li, X., Lin, et al
2024; 95 (12)
- **Terawatt-scale attosecond X-ray pulses from a cascaded superradiant free-electron laser** *NATURE PHOTONICS*
Franz, P., Li, S., Driver, T., Robles, R. R., Cesar, D., Isele, E., Guo, Z., Wang, J., Duris, J. P., Larsen, K., Glowonia, J. M., Cheng, X., Hoffmann, et al
2024
- **Experimental demonstration of attosecond pump-probe spectroscopy with an X-ray free-electron laser** *NATURE PHOTONICS*
Guo, Z., Driver, T., Beauvarlet, S., Cesar, D., Duris, J., Franz, P. L., Alexander, O., Bohler, D., Bostedt, C., Averbukh, V., Cheng, X., Dimauro, L. F., Doumy, et al
2024
- **Massive Scale Data Analytics at LCLS-II**
Thayer, J., Chen, Z., Claus, R., Damiani, D., Ford, C., Dubrovin, M., Elmir, V., Kroeger, W., Li, X., Marchesini, S., Mariani, V., Melcchiori, R., Nelson, et al
edited by Espinal, DeVita, R., Laycock, P., Shadura, O.
E D P SCIENCES.2024
- **Investigating charge-up and fragmentation dynamics of oxygen molecules after interaction with strong X-ray free-electron laser pulses.** *Physical chemistry chemical physics : PCCP*
Kastirke, G., Ota, F., Rezvan, D. V., Schöffler, M. S., Weller, M., Rist, J., Boll, R., Anders, N., Baumann, T. M., Eckart, S., Erk, B., De Fanis, A., Fehre, et al
2022; 24 (44): 27121-27127
- **The DREAM Endstation at the Linac Coherent Light Source** *APPLIED SCIENCES-BASEL*
Walter, P., Holmes, M., Obaid, R., Amores, L., Cheng, X., Cryan, J. P., Glowonia, J. M., Li, X., Lin, M., Ng, M., Robinson, J., Shivaram, N., Yin, et al
2022; 12 (20)
- **Strong-Field-Induced Coulomb Explosion Imaging of Tribromomethane.** *The journal of physical chemistry letters*
Bhattacharyya, S., Borne, K., Ziaee, F., Pathak, S., Wang, E., Venkatachalam, A. S., Li, X., Marshall, N., Carnes, K. D., Fehrenbach, C. W., Severt, T., Ben-Itzhak, I., Rudenko, et al
2022; 13 (25): 5845-5853

- **Resonance-enhanced x-ray multiple ionization of a polyatomic molecule** *PHYSICAL REVIEW A*
Li, X., Rudenko, A., Mazza, T., Roerig, A., Anders, N., Baumann, T. M., Eckart, S., Erk, B., De Fanis, A., Fehre, K., Doerner, R., Foucar, L., Grundmann, et al
2022; 105 (5)
- **X-ray multiphoton-induced Coulomb explosion images complex single molecules** *NATURE PHYSICS*
Boll, R., Schaefer, J. M., Richard, B., Fehre, K., Kastirke, G., Jurek, Z., Schoeffler, M. S., Abdullah, M. M., Anders, N., Baumann, T. M., Eckart, S., Erk, B., De Fanis, et al
2022; 18 (4): 423-+
- **Coulomb explosion imaging of small polyatomic molecules with ultrashort x-ray pulses** *PHYSICAL REVIEW RESEARCH*
Li, X., Rudenko, A., Schoeffler, M. S., Anders, N., Baumann, T. M., Eckart, S., Erk, B., De Fanis, A., Fehre, K., Doerner, R., Foucar, L., Grundmann, S., Grychtol, et al
2022; 4 (1)
- **The X-ray Focusing System at the Time-Resolved AMO Instrument** *Synchrotron Radiation News*
Seaberg, M., et al
2022; 35 (2): 20-28
- **Inner-Shell-Ionization-Induced Femtosecond Structural Dynamics of Water Molecules Imaged at an X-Ray Free-Electron Laser** *PHYSICAL REVIEW X*
Jahnke, T., Guillemin, R., Inhester, L., Son, S., Kastirke, G., Ilchen, M., Rist, J., Trabert, D., Melzer, N., Anders, N., Mazza, T., Boll, R., De Fanis, et al
2021; 11 (4)
- **Simple model for sequential multiphoton ionization by ultraintense x rays** *PHYSICAL REVIEW A*
Li, X., Boll, R., Rolles, D., Rudenko, A.
2021; 104 (3)
- **Pulse Energy and Pulse Duration Effects in the Ionization and Fragmentation of Iodomethane by Ultraintense Hard X Rays.** *Physical review letters*
Li, X., Inhester, L., Robotjazi, S. J., Erk, B., Boll, R., Hanasaki, K., Toyota, K., Hao, Y., Bomme, C., Rudek, B., Foucar, L., Southworth, S. H., Lehmann, et al
2021; 127 (9): 093202
- **Electron-ion coincidence measurements of molecular dynamics with intense X-ray pulses.** *Scientific reports*
Li, X., Inhester, L., Osipov, T., Boll, R., Coffee, R., Cryan, J., Gatton, A., Gorkhover, T., Hartman, G., Ilchen, M., Knie, A., Lin, M., Minitti, et al
2021; 11 (1): 505
- **Differentiating and Quantifying Gas-Phase Conformational Isomers Using Coulomb Explosion Imaging.** *The journal of physical chemistry letters*
Pathak, S., Obaid, R., Bhattacharyya, S., Bürger, J., Li, X., Tross, J., Severt, T., Davis, B., Bilodeau, R. C., Trallero-Herrero, C. A., Rudenko, A., Berrah, N., Rolles, et al
2020; 11 (23): 10205-10211
- **Double Core-Hole Generation in O₂ Molecules Using an X-Ray Free-Electron Laser: Molecular-Frame Photoelectron Angular Distributions.** *Physical review letters*
Kastirke, G., Schöffler, M. S., Weller, M., Rist, J., Boll, R., Anders, N., Baumann, T. M., Eckart, S., Erk, B., De Fanis, A., Fehre, K., Gatton, A., Grundmann, et al
2020; 125 (16): 163201
- **Electronic Population Transfer via Impulsive Stimulated X-Ray Raman Scattering with Attosecond Soft-X-Ray Pulses.** *Physical review letters*
O'Neal, J. T., Champenois, E. G., Oberli, S., Obaid, R., Al-Haddad, A., Barnard, J., Berrah, N., Coffee, R., Duris, J., Galinis, G., Garratt, D., Glowia, J. M., Haxton, et al
2020; 125 (7): 073203
- **Photoelectron Diffraction Imaging of a Molecular Breakup Using an X-Ray Free-Electron Laser** *PHYSICAL REVIEW X*
Kastirke, G., Schoeffler, M. S., Weller, M., Rist, J., Boll, R., Anders, N., Baumann, T. M., Eckart, S., Erk, B., De Fanis, A., Fehre, K., Gatton, A., Grundmann, et al
2020; 10 (2)
- **State-selective dissociation dynamics of an oxygen molecular ion studied with single-harmonic pump and infrared-probe pulses** *PHYSICAL REVIEW A*

Malakar, Y., Wilhelm, F., Trabert, D., Raju, K. P., Li, X., Pearson, W. L., Cao, W., Kaderiya, B., Ben-Itzhak, I., Rudenko, A.
2018; 98 (1)

- **Femtosecond response of polyatomic molecules to ultra-intense hard X-rays.** *Nature*

Rudenko, A., Inhester, L., Hanasaki, K., Li, X., Robotjazi, S. J., Erk, B., Boll, R., Toyota, K., Hao, Y., Vendrell, O., Bomme, C., Savelyev, E., Rudek, et al
2017; 546 (7656): 129-132