Stanford

Andrew Lee Aquila

Staff Scientist, SLAC National Accelerator Laboratory

Bio

BIO

Andrew Aquila is an X-ray physicist, having started my education in synchrotron radiation science with a focus on soft X-ray spectroscopy. Since 2014 he has worked at the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory. His inserts are in advancing X-ray techniques in imaging, and spectroscopy with a focus in nonlinear X-ray methods and X-ray quantum imaging.

CURRENT ROLE AT STANFORD

Tender X-ray Instrument (TXI) lead - Andrew Aquila leads one of the scientific instruments at LCLS. TXI focuses on the tender X-ray spectrum (2 keV to 7 keV), with dedicated instrumentation for laser pumped tender spectroscopy, forward scattering and X-ray pump/X-ray probe methods.

EDUCATION AND CERTIFICATIONS

- PhD, UC Berkeley , Applied Science & Technology (2009)
- BS, UC Berkeley , Engineering Physics (2004)

LINKS

- LCLS: https://lcls.slac.stanford.edu/

Publications

PUBLICATIONS

- **X-ray diffraction of metastable structures from supercooled liquid hydrogen.** *Scientific reports*
  Fletcher, L. B., Levitan, A. L., McBride, E. E., Kim, J. B., Alves, E. P., Aquila, A., Frost, M., Goede, S., King, G., Lane, T. J., Liang, M., MacDonald, M. J., Ofori-Okai, et al
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- **Development of spinning-disk solid sample delivery system for high-repetition rate x-ray free electron laser experiments.** *The Review of scientific instruments*
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- **Optical control of ultrafast structural dynamics in a fluorescent protein.** *Nature chemistry*
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- **Regioselective, catalytic 1,1-difluorination of enynes** *NATURE CHEMISTRY*
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- **Microstructure and crystal order during freezing of supercooled water drops.** *Nature*
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- **Revealing core-valence interactions in solution with femtosecond X-ray pump X-ray probe spectroscopy.** *Nature communications*
  Weakly, R. B., Liekhus-Schmaltz, C. E., Poulter, B. I., Biasin, E., Alonso-Mori, R., Aquila, A., Boutet, S., Fuller, F. D., Ho, P. J., Kroll, T., Loe, C. M., Lutman, A., Zhu, et al
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- **Nonsequential two-photon absorption in solid Ge irradiated by an intense x-ray free-electron-laser pulse** *PHYSICAL REVIEW A*
  Wirok-Stoletow, S., Jin, R., Kolbasova, D., Son, S., Aquila, A., Santra, R.
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- **Observations of phase changes in monoolein during high viscous injection.** *Journal of synchrotron radiation*
  Wells, D. J., Berntsen, P., Balaur, E., Kewish, C. M., Adams, P., Aquila, A., Binns, J., Boutet, S., Broomhall, H., Caleman, C., Christofferson, A., Conn, C. E., Dahlqvist, et al
  2022; 29 (Pt 3): 602-614

- **Erratum: An advanced workflow for single-particle imaging with the limited data at an X-ray free-electron laser. Corrigendum.** *IUCrJ*
  Assalauova, D., Kim, Y. Y., Bobkov, S., Khubbutdinov, R., Rose, M., Alvarez, R., Andreasson, J., Balaur, E., Contreras, A., DeMirci, H., Gelisio, L., Hajdu, J., Hunter, et al
  2022; 9 (Pt 2): 328

- **Chemical crystallography by serial femtosecond X-ray diffraction.** *Nature*
  Schriber, E. A., Paley, D. W., Bolotovsky, R., Rosenberg, D. J., Sierra, R. G., Aquila, A., Mendez, D., Poitevin, F., Blaschke, J. P., Bhowmick, A., Kelly, R. P., Hunter, M., Hayes, et al
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- **Ultrafast x-ray pump x-ray probe transient absorption spectroscopy: A computational study and proposed experiment probing core-valence electronic correlations in solvated complexes.** *The Journal of chemical physics*
  Liekhus-Schmaltz, C. E., Ho, P. J., Weakly, R. B., Aquila, A., Schoenlein, R. W., Khalil, M., Govind, N.
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- **Observation of shock-induced protein crystal damage during megahertz serial femtosecond crystallography** *PHYSICAL REVIEW RESEARCH*
  Gruenbein, M. L., Foucar, L., Gorel, A., Hilpert, M., Kloos, M., Nass, K., Kovacs, G., Roome, C. M., Shoeman, R. L., Stricker, M., Carbajo, S., Colocho, W., Gilevich, et al
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- **Effect of X-ray free-electron laser-induced shockwaves on haemoglobin microcrystals delivered in a liquid jet.** *Nature communications*
  Grünbein, M. L., Gorel, A. n., Foucar, L. n., Carbajo, S. n., Colocho, W. n., Gilevich, S. n., Hartmann, E. n., Hilpert, M. n., Hunter, M. n., Kloos, M. n., Koglin, J. E., Lane, T. J., Lewandowski, et al
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- **An advanced workflow for single-particle imaging with the limited data at an X-ray free-electron laser.** *IUCrJ*
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- **Harnessing the power of an X-ray laser for serial crystallography of membrane proteins crystallized in lipidic cubic phase.** *IUCrJ*
  Lee, M., Geiger, J., Ishchenko, A., Han, G. W., Barty, A., White, T. A., Gati, C., Batyuk, A., Hunter, M. S., Aquila, A., Boutet, S., Weierstall, U., Cherezov, et al
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- **Structural dynamics in proteins induced by and probed with X-ray free-electron laser pulses.** *Nature communications*
  Nass, K., Gorel, A., Abdullah, M. M., V Martin, A., Kloos, M., Marinelli, A., Aquila, A., Barends, T. R., Decker, F., Bruce Doak, R., Foucar, L., Hartmann, E., Hilpert, et al
  2020; 11 (1): 1814

- **Diffraction data from aerosolized Coliphage PR772 virus particles imaged with the Linac Coherent Light Source.** *Scientific data*
  Li, H. n., Nazari, R. n., Abbey, B. n., Alvarez, R. n., Aquila, A. n., Ayyer, K. n., Barty, A. n., Berntsen, P. n., Bielecki, J. n., Pietrini, A. n., Bucher, M. n., Carini, G. n., Chapman, et al
  2020; 7 (1): 404

- **Low-signal limit of X-ray single particle diffractive imaging** *OPTICS EXPRESS*
  Ayyer, K., Morgan, A. J., Aquila, A., DeMirci, H., Hogue, B. G., Kirian, R. A., Xavier, P., Yoon, C., Chapman, H. N., Barty, A.
  2019; 27 (26): 37816–33

- **Wavefront sensing at X-ray free-electron lasers.** *Journal of synchrotron radiation*
  Seaberg, M., Cojocaru, R., Berujon, S., Ziegler, E., Jaggi, A., Krempasky, J., Seiboth, F., Aquila, A., Liu, Y., Sakdinawat, A., Lee, H. J., Flechsig, U., Patthey, et al
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- **Generation of high-intensity ultrasound through shock propagation in liquid jets** *PHYSICAL REVIEW FLUIDS*
  Blaj, G., Liang, M., Aquila, A. L., Willmott, P. R., Koglin, J. E., Sierra, R. G., Robinson, J. S., Boutet, S., Stan, C. A.
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- **The Macromolecular Femtosecond Crystallography Instrument at the Linac Coherent Light Source** *JOURNAL OF SYNCHROTRON RADIATION*
  Sierra, R. G., Batyuk, A., Sun, Z., Aquila, A., Hunter, M. S., Lane, T. J., Liang, M., Yoon, C., Alonso-Mori, R., Armenta, R., Castagna, J., Hollenbeck, M., Osier, et al
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- **Evaluation of the performance of classification algorithms for XFEL single-particle imaging data** *IUCRJ*
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  Liu, Y., Seaberg, M., Zhu, D., Krzywinski, J., Seiboth, F., Hardin, C., Cocco, D., Aquila, A., Nagler, B., Lee, H., Boutet, S., Feng, Y., Ding, et al
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- **Deconvoluting the isotropic and anisotropic ultrafast x-ray scattering of gas-phase N-methylmorpholine following Rydberg excitation**
  Stankus, B., Ruddock, J., Yong, H., Zotev, N., Bellshaw, D., Lane, T., Boutet, S., Liang, M., Carbajo, S., Robinson, J., Koglin, J., Aquila, A., Zhang, et al
  AMER CHEMICAL SOC.2018

- **Ultrafast nonthermal heating of water initiated by an X-ray Free-Electron Laser** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Beyerlein, K. R., Jonsson, H., Alonso-Mori, R., Aquila, A., Barty, S., Barty, A., Bean, R., Koglin, J. E., Messerschmidt, M., Ragazzon, D., Sokaras, D., Williams, G. J., Hau-Riege, et al
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- **Stimulated X-Ray Emission Spectroscopy in Transition Metal Complexes** *PHYSICAL REVIEW LETTERS*
  Kroll, T., Weninger, C., Alonso-Mori, R., Sokaras, D., Zhu, D., Mercadier, L., Majety, V. P., Marinelli, A., Lutman, A., Guetg, M. W., Decker, F., Boutet, S., Aquila, et al
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- **Femtosecond X-ray diffraction from an aerosolized beam of protein nanocrystals** *JOURNAL OF APPLIED CRYSTALLOGRAPHY*

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- **Single Molecule Imaging Using X-ray Free Electron Lasers** *X-ray Free Electron Lasers*

  Aquila, A., Barty, A.

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- **Developments Towards Imaging Nanoscale Biology with XFELs: Some Recent Examples and a Glance to the Future** *Microscopy and Microanalysis*

  Mancuso, A. P., Aquila, A., Bean, R., Bielecki, J., Fortmann-Grote, C., Giewekemeyer, K., Kim, Y., Kurta, R., Letrun, R., Mehrjoo, M., Messerschmidt, M., Mills, G., Round, et al

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- **X-ray Emission Spectroscopy at X-ray Free Electron Lasers: Limits to Observation of the Classical Spectroscopic Response for Electronic Structure Analysis.** *The journal of physical chemistry letters*

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- **Chromophore twisting in the excited state of a photoswitchable fluorescent protein captured by time-resolved serial femtosecond crystallography** *NATURE CHEMISTRY*

  Coquelle, N., Sliwa, M., Woodhouse, J., Schiro, G., Adam, V., Aquila, A., Barends, T. R. M., Boutet, S., Byrdin, M., Carbajo, S., De la Mora, E., Doak, R., Feliks, et al

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  Wojtas, D. H., Ayyer, K., Liang, M., Mossou, E., Romoli, F., Seuring, C., Beyerlein, K. R., Bean, R. J., Morgan, A. J., Oberthuer, D., Fleckenstein, H., Heymann, M., Gati, et al

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  Nagler, B., Aquila, A., Boutet, S., Galtier, E. C., Hashim, A., Hunter, M. S., Liang, M., Sakdinawat, A. E., Schroer, C. G., Schropp, A., Seaberg, M. H., Seiboth, F., van Driel, et al

  2017; 7: 13698

- **Correlations in Scattered X-Ray Laser Pulses Reveal Nanoscale Structural Features of Viruses** *PHYSICAL REVIEW LETTERS*

  Kurta, R. P., Donatelli, J. J., Yoon, C., Berntsen, P., Bielecki, J., Daurer, B. J., DeMirci, H., Fromme, P., Hantke, M., Maia, F. C., Munke, A., Nettelblad, C., Pande, et al

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- **Conformational landscape of a virus by single-particle X-ray scattering** *NATURE METHODS*

  Hosseinizadeh, A., Mashayekhi, G., Copperman, J., Schwander, P., Dashti, A., Sepehr, R., Fung, R., Schmidt, M., Yoon, C., Hogue, B. G., Williams, G. J., Aquila, A., Ourmazd, et al

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- **Impact of B4C co-sputtering on structure and optical performance of Cr/Sc multilayer X-ray mirrors** *OPTICS EXPRESS*

  Ghafoor, N., Eriksson, F., Aquila, A., Gullikson, E., Schaefers, F., Greczynski, G., Birch, J.

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- **Structural enzymology using X-ray free electron lasers.** *Structural dynamics*

  Kupitz, C., Olmos, J. L., Holl, M., Tremblay, L., Pande, K., Pandey, S., Oberthür, D., Hunter, M., Liang, M., Aquila, A., Tenboer, J., Calvey, G., Katz, et al

  2017; 4 (4): 044003-?

- **Numerical simulations of the hard X-ray pulse intensity distribution at the Linac Coherent Light Source** *JOURNAL OF SYNCHROTRON RADIATION*

  Pardini, T., Aquila, A., Boutet, S., Cocco, D., Hau-Riege, S. P.

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- **Coherent soft X-ray diffraction imaging of coliphage PR772 at the Linac coherent light source** *SCIENTIFIC DATA*

Reddy, H. K. N., Yoon, C., Aquila, A., Awel, S., Ayyer, K., Barty, A., Berntsen, P., Bielecki, J., Bobkov, S., Bucher, M., Carini, G. A., Carron, S., Chapman, et al

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- **Double-flow focused liquid injector for efficient serial femtosecond crystallography (vol 7, 44628, 2017)** *SCIENTIFIC REPORTS*

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  Yoon, C. H., Demirci, H., Sierra, R. G., Dao, E. H., Ahmadi, R., Aksit, F., Aquila, A. L., Batyuk, A., Ciftci, H., Guillet, S., Hayes, M. J., Hayes, B., Lane, et al

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- **Atomic structure of granulin determined from native nanocrystalline granulovirus using an X-ray free-electron laser** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

  Gati, C., Oberthuer, D., Yefanov, O., Bunker, R. D., Stellato, F., Chiu, E., Yeh, S., Aquila, A., Basu, S., Bean, R., Beyerlein, K. R., Botha, S., Boutet, et al

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- **Selenium single-wavelength anomalous diffraction de novo phasing using an X-ray-free electron laser.** *Nature communications*

  Hunter, M. S., Yoon, C. H., Demirci, H., Sierra, R. G., Dao, E. H., Ahmadi, R., Aksit, F., Aquila, A. L., Ciftci, H., Guillet, S., Hayes, M. J., Lane, T. J., Liang, et al

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- **Liquid explosions induced by X-ray laser pulses** *NATURE PHYSICS*

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- **Native phasing of x-ray free-electron laser data for a G protein-coupled receptor** *SCIENCE ADVANCES*

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- **Design of the mirror optical systems for coherent diffractive imaging at the SPB/SFX instrument of the European XFEL** *JOURNAL OF OPTICS*

  Bean, R. J., Aquila, A., Samoylova, L., Mancuso, A. P.

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- **Negative Pressures and Spallation in Water Drops Subjected to Nanosecond Shock Waves** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*

  Stan, C. A., Willmott, P. R., Stone, H. A., Koglin, J. E., Liang, M., Aquila, A. L., Robinson, J. S., Gumerlock, K. L., Blaj, G., Sierra, R. G., Boutet, S., Guillet, S. A., Curtis, et al

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- **Protein structure determination by single-wavelength anomalous diffraction phasing of X-ray free-electron laser data** *IUCRJ*

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- **Femtosecond and nanometre visualization of structural dynamics in superheated nanoparticles** *NATURE PHOTONICS*
  Gorkhover, T., Schorb, S., Coffee, R., Adolph, M., Foucar, L., Rupp, D., Aquila, A., Bozek, J. D., Epp, S. W., Erk, B., Gumprecht, L., Holmegaard, L., Hartmann, et al
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- **Coherent diffraction of single Rice Dwarf virus particles using hard X-rays at the Linac Coherent Light Source.** *Scientific data*
  Munke, A., Andreasson, J., Aquila, A., Awel, S., Ayyer, K., Barty, A., Bean, R. J., Berntsen, P., Bielecki, J., Boutet, S., Bucher, M., Chapman, H. N., Daurer, et al
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  Ekeberg, T., Svenda, M., Seibert, M. M., Abergel, C., Maia, F. R., Seltzer, V., Deponte, D. P., Aquila, A., Andreasson, J., Iwan, B., Jönsson, O., Westphal, D., Odic, et al
  2016; 3: 160060-?

- **Concentric-flow electrokinetic injector enables serial crystallography of ribosome and photosystem II** *NATURE METHODS*
  Sierra, R. G., Gati, C., Laksmono, H., Dao, E. H., Gul, S., Fuller, F., Kern, J., Chatterjee, R., Ibrahim, M., Brewster, A. S., Young, I. D., Michels-Clark, T., Aquila, et al
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  Giewekemeyer, K., Hackenberg, C., Aquila, A., Wilke, R. N., Groves, M. R., Jordanova, R., Lamzin, V. S., Borchers, G., Saksl, K., Zozulya, A. V., Sprung, M., Mancuso, A. P.
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  Barends, T. R. M., Foucar, L., Ardevol, A., Nass, K., Aquila, A., Botha, S., Doak, R., Falahati, K., Hartmann, E., Hilpert, M., Heinz, M., Hoffmann, M. C., Koefinger, et al
  2015; 350 (6259): 445–50

- **The linac coherent light source single particle imaging road map** *STRUCTURAL DYNAMICS*
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  Conrad, C. E., Basu, S., James, D., Wang, D., Schaffer, A., Roy-Chowdhury, S., Zatsepin, N. A., Aquila, A., Coe, J., Gati, C., Hunter, M. S., Koglin, J. E., Kupitz, et al
  2015; 2: 421–30

- **Fluence thresholds for grazing incidence hard x-ray mirrors** *APPLIED PHYSICS LETTERS*
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- **High numerical aperture multilayer Laue lenses** *SCIENTIFIC REPORTS*
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- **The Coherent X-ray Imaging instrument at the Linac Coherent Light Source** *JOURNAL OF SYNCHROTRON RADIATION*
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