

## Andrew Lee Aquila

Staff Scientist, SLAC National Accelerator Laboratory

### Publications

---

#### PUBLICATIONS

- **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  
2021; 3 (1)
- **An advanced workflow for single-particle imaging with the limited data at an X-ray free-electron laser.** *IUCrJ*  
Assalauova, D., Kim, Y. Y., Bobkov, S., Khubbutdinov, R., Rose, M., Alvarez, R., Andreasson, J., Balaur, E., Contreras, A., DeMirici, H., Gelisio, L., Hajdu, J., Hunter, et al  
2020; 7 (Pt 6): 1102–13
- **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  
2020; 7 (Pt 6): 976–84
- **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., DeMirici, 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  
2019; 26 (Pt 4): 1115–26
- **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.  
2019; 4 (4)
- **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  
2019; 26: 346–57
- **Evaluation of the performance of classification algorithms for XFEL single-particle imaging data.** *IUCrJ*  
Shi, Y., Yin, K., Tai, X., DeMirici, H., Hosseinizadeh, A., Hogue, B. G., Li, H., Ourmazd, A., Schwander, P., Vartanyants, I. A., Yoon, C. H., Aquila, A., Liu, et al  
2019; 6 (Pt 2): 331–40
- **The Macromolecular Femtosecond Crystallography Instrument at the Linac Coherent Light Source.** *Journal of synchrotron radiation*

- Sierra, R. G., Batyuk, A. n., Sun, Z. n., Aquila, A. n., Hunter, M. S., Lane, T. J., Liang, M. n., Yoon, C. H., Alonso-Mori, R. n., Armenta, R. n., Castagna, J. C., Hollenbeck, M. n., Osier, et al  
2019; 26 (Pt 2): 346–57
- **Single-particle imaging without symmetry constraints at an X-ray free-electron laser** *IUCRJ*  
Rose, M., Bobkov, S., Ayer, K., Kurta, R. P., Dzhigaev, D., Kim, Y., Morgan, A. J., Yoon, C., Westphal, D., Bielecki, J., Sellberg, J. A., Williams, G., Maia, et al  
2018; 5: 727–36
  - **High-accuracy wavefront sensing for x-ray free electron lasers** *OPTICA*  
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  
2018; 5 (8): 967–75
  - **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  
2018; 115 (22): 5652–57
  - **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  
2018; 120 (13): 133203
  - **Femtosecond X-ray diffraction from an aerosolized beam of protein nanocrystals** *JOURNAL OF APPLIED CRYSTALLOGRAPHY*  
Awel, S., Kirian, R. A., Wiedorn, M. O., Beyerlein, K. R., Roth, N., Horke, D. A., Oberthuer, D., Knoska, J., Mariani, V., Morgan, A., Adriano, L., Tolstikova, A., Xavier, et al  
2018; 51: 133–39
  - **Single Molecule Imaging Using X-ray Free Electron Lasers** *X-ray Free Electron Lasers*  
Aquila, A., Barty, A.  
Springer International Publishing.2018: 401–426
  - **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  
2018; 24: 76–77
  - **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*  
Jensen, S. n., Sullivan, B. T., Hartzler, D. A., Meza Aguilar, J. n., Awel, S. n., Bajt, S. n., Basu, S. n., Bean, R. n., Chapman, H. n., Conrad, C. n., Frank, M. n., Fromme, R. n., Martin-Garcia, et al  
2018
  - **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. M., Boutet, S., Byrdin, M., Carbajo, S., De la Mora, E., Doak, R., Feliks, et al  
2018; 10 (1): 31–37
  - **Analysis of XFEL serial diffraction data from individual crystalline fibrils** *IUCRJ*  
Wojtas, D. H., Ayer, 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  
2017; 4: 795–811
  - **Focal Spot and Wavefront Sensing of an X-Ray Free Electron laser using Ronchi shearing interferometry** *SCIENTIFIC REPORTS*  
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., DeMirici, H., Fromme, P., Hantke, M., Maia, F. C., Munke, A., Nettelblad, C., Pande, et al  
2017; 119 (15): 158102
- **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  
2017; 14 (9): 877-+
- **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., Schaefer, F., Greczynski, G., Birch, J.  
2017; 25 (15): 18274-87
- **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.  
2017; 24: 738-43
- **Coherent soft X-ray diffraction imaging of coliphage PR772 at the Linac coherent light source** *SCIENTIFIC DATA*  
Reddy, H. 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  
2017; 4: 170079
- **Double-flow focused liquid injector for efficient serial femtosecond crystallography (vol 7, 44628, 2017)** *SCIENTIFIC REPORTS*  
Oberthuer, D., Knoska, J., Wiedorn, M. O., Beyerlein, K. R., Bushnell, D. A., Kovaleva, E. G., Heymann, M., Gumprecht, L., Kirian, R. A., Barty, A., Mariani, V., Tolstikova, A., Adriano, et al  
2017; 7: 46846
- **Se-SAD serial femtosecond crystallography datasets from selenobiotinyl-streptavidin** *SCIENTIFIC DATA*  
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  
2017; 4
- **Double-flow focused liquid injector for efficient serial femtosecond crystallography** *SCIENTIFIC REPORTS*  
Oberthuer, D., Knoska, J., Wiedorn, M. O., Beyerlein, K. R., Bushnell, D. A., Kovaleva, E. G., Heymann, M., Gumprecht, L., Kirian, R. A., Barty, A., Mariani, V., Tolstikova, A., Adriano, et al  
2017; 7: 44628
- **Atomic structure of granulins 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  
2017; 114 (9): 2247-52
- **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  
2016; 7: 13388-?
- **Liquid explosions induced by X-ray laser pulses** *NATURE PHYSICS*  
Stan, C. A., Milathianaki, D., Laksmono, H., Sierra, R. G., McQueen, T. A., Messerschmidt, M., Williams, G. J., Koglin, J. E., Lane, T. J., Hayes, M. J., Guillet, S. A., Liang, M., Aquila, et al  
2016; 12 (10): 966-971
- **Native phasing of x-ray free-electron laser data for a G protein-coupled receptor** *SCIENCE ADVANCES*  
Batyuk, A., Galli, L., Ishchenko, A., Han, G., Gati, C., Popov, P. A., Lee, M., Stauch, B., White, T. A., Barty, A., Aquila, A., Hunter, M. S., Liang, et al  
2016; 2 (9): e1600292
- **Open data set of live cyanobacterial cells imaged using an X-ray laser** *SCIENTIFIC DATA*

- van der Schot, G., Svenda, M., Maia, F. C., Hantke, M. F., DePonte, D. P., Seibert, M., Aquila, A., Schulz, J., Kirian, R. A., Liang, M., Stellato, F., Bari, S., Iwan, et al  
2016; 3: 160058
- **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.  
2016; 18 (7)
  - **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  
2016; 7 (11): 2055-2062
  - **Protein structure determination by single-wavelength anomalous diffraction phasing of X-ray free-electron laser data** *IUCRJ*  
Nass, K., Meinhart, A., Barends, T. M., Foucar, L., Gorel, A., Aquila, A., Botha, S., Doak, R., Koglin, J., Liang, M., Shoeman, R. L., Williams, G., Boutet, et al  
2016; 3: 180-91
  - **Macromolecular diffractive imaging using imperfect crystals** *NATURE*  
Ayyer, K., Yefanov, O. M., Oberthuer, D., Roy-Chowdhury, S., Galli, L., Mariani, V., Basu, S., Coe, J., Conrad, C. E., Fromme, R., Schaffer, A., Droener, K., James, et al  
2016; 530 (7589): 202-+
  - **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  
2016; 10 (2): 93-+
  - **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  
2016; 3: 160064-?
  - **Single-shot diffraction data from the Mimivirus particle using an X-ray free-electron laser.** *Scientific data*  
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  
2016; 13 (1): 59-?
  - **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  
2016; 13 (1): 59-62
  - **Tomography of a Cryo-immobilized Yeast Cell Using Ptychographic Coherent X-Ray Diffractive Imaging** *BIOPHYSICAL JOURNAL*  
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.  
2015; 109 (9): 1986-95
  - **Direct observation of ultrafast collective motions in CO myoglobin upon ligand dissociation** *SCIENCE*  
Barends, T. 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*  
Aquila, A., Barty, A., Bostedt, C., Boutet, S., Carini, G., Deponte, D., DRELL, P., Doniach, S., Downing, K. H., Earnest, T., Elmlund, H., Elser, V., Guehr, et al  
2015; 2 (4)
  - **Serial femtosecond X-ray diffraction of enveloped virus microcrystals** *STRUCTURAL DYNAMICS*

- Lawrence, R. M., Conrad, C. E., Zatsepin, N. A., Grant, T. D., Liu, H., James, D., Nelson, G., Subramanian, G., Aquila, A., Hunter, M. S., Liang, M., Boutet, S., Coe, et al  
2015; 2 (4): 041720
- **A novel inert crystal delivery medium for serial femtosecond crystallography** *IUCRJ*  
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*  
Aquila, A., Sobierajski, R., Ozkan, C., Hajkova, V., Burian, T., Chalupsky, J., Juha, L., Stoermer, M., Bajt, S., Klepka, M. T., Dluzewski, P., Morawiec, K., Ohashi, et al  
2015; 106 (24)
  - **High numerical aperture multilayer Laue lenses** *SCIENTIFIC REPORTS*  
Morgan, A. J., Prasciolu, M., Andrejczuk, A., Krzywinski, J., Meents, A., Pennicard, D., Graafsma, H., Barty, A., Bean, R. J., Barthelmess, M., Oberthuer, D., Yefanov, O., Aquila, et al  
2015; 5: 9892
  - **The Coherent X-ray Imaging instrument at the Linac Coherent Light Source** *JOURNAL OF SYNCHROTRON RADIATION*  
Liang, M., Williams, G. J., Messerschmidt, M., Seibert, M., Montanez, P. A., Hayes, M., Milathianaki, D., Aquila, A., Hunter, M. S., Koglin, J. E., Schafer, D. W., Guillet, S., Busse, et al  
2015; 22: 514–19
  - **Indications of radiation damage in ferredoxin microcrystals using high-intensity X-FEL beams** *JOURNAL OF SYNCHROTRON RADIATION*  
Nass, K., Foucar, L., Barends, T. M., Hartmann, E., Botha, S., Shoeman, R. L., Doak, R., Alonso-Mori, R., Aquila, A., Bajt, S., Barty, A., Bean, R., Beyerlein, et al  
2015; 22: 225–38
  - **Imaging single cells in a beam of live cyanobacteria with an X-ray laser** *NATURE COMMUNICATIONS*  
van der Schot, G., Svenda, M., Maia, F. C., Hantke, M., DePonte, D. P., Seibert, M., Aquila, A., Schulz, J., Kirian, R., Liang, M., Stellato, F., Iwan, B., Andreasson, et al  
2015; 6: 5704
  - **Ultrafast self-gating Bragg diffraction of exploding nanocrystals in an X-ray laser** *OPTICS EXPRESS*  
Caleman, C., Timneanu, N., Martin, A. V., Jonsson, H., Aquila, A., Barty, A., Scott, H. A., White, T. A., Chapman, H. N.  
2015; 23 (2): 1213–31
  - **Explosion dynamics of sucrose nanospheres monitored by time of flight spectrometry and coherent diffractive imaging at the split-and-delay beam line of the FLASH soft X-ray laser** *OPTICS EXPRESS*  
Rath, A. D., Timneanu, N., Maia, F. C., Bielecki, J., Fleckenstein, H., Iwan, B., Svenda, M., Hasse, D., Carlsson, G., Westphal, D., Muhlig, K., Hantke, M., Ekeberg, et al  
2014; 22 (23): 28914–25
  - **Serial time-resolved crystallography of photosystem II using a femtosecond X-ray laser.** *Nature*  
Kupitz, C., Basu, S., Grotjohann, I., Fromme, R., Zatsepin, N. A., Rendek, K. N., Hunter, M. S., Shoeman, R. L., White, T. A., Wang, D., James, D., Yang, J. H., Cobb, et al  
2014; 513 (7517): 261-5
  - **Serial time-resolved crystallography of photosystem II using a femtosecond X-ray laser** *NATURE*  
Kupitz, C., Basu, S., Grotjohann, I., Fromme, R., Zatsepin, N. A., Rendek, K. N., Hunter, M. S., Shoeman, R. L., White, T. A., Wang, D., James, D., Yang, J., Cobb, et al  
2014; 513 (7517): 261-?
  - **Visualizing a protein quake with time-resolved X-ray scattering at a free-electron laser** *NATURE METHODS*  
Arlund, D., Johansson, L. C., Wickstrand, C., Barty, A., Williams, G. J., Malmerberg, E., Davidsson, J., Milathianaki, D., DePonte, D. P., Shoeman, R. L., Wang, D., James, D., Katona, et al  
2014; 11 (9): 923–26
  - **High-dynamic-range coherent diffractive imaging: ptychography using the mixed-mode pixel array detector** *JOURNAL OF SYNCHROTRON RADIATION*  
Giewekemeyer, K., Philipp, H. T., Wilke, R. N., Aquila, A., Osterhoff, M., Tate, M. W., Shanks, K. S., Zozulya, A. V., Salditt, T., Gruner, S. M., Mancuso, A. P.  
2014; 21: 1167–74

- **Expression, purification and crystallization of CTB-MPR, a candidate mucosal vaccine component against HIV-1** *IUCRJ*  
Lee, H., Cherni, I., Yu, H., Fromme, R., Doran, J. D., Grotjohan, I., Mittman, M., Basu, S., Deb, A., Doerner, K., Aquila, A., Barty, A., Boutet, et al  
2014; 1: 305–17
- **Femtosecond x-ray photoelectron diffraction on gas-phase dibromobenzene molecules** *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*  
Rolles, D., Boll, R., Adolph, M., Aquila, A., Bostedt, C., Bozek, J. D., Chapman, H. N., Coffee, R., Coppola, N., Decleva, P., Delmas, T., Epp, S. W., Erk, et al  
2014; 47 (12)
- **Investigation of surface topology of printed nanoparticle layers using wide-angle low-Q scattering** *JOURNAL OF SYNCHROTRON RADIATION*  
Jonah, E. O., Haerting, M., Gullikson, E., Aquila, A., Britton, D. T.  
2014; 21: 547–53
- **X-Ray Diffraction from Isolated and Strongly Aligned Gas-Phase Molecules with a Free-Electron Laser** *PHYSICAL REVIEW LETTERS*  
Kuepper, J., Stern, S., Holmegaard, L., Filsinger, F., Rouzee, A., Rudenko, A., Johnsson, P., Martin, A. V., Adolph, M., Aquila, A., Bajt, S., Barty, A., Bostedt, et al  
2014; 112 (8)
- **Automated identification and classification of single particle serial femtosecond X-ray diffraction data** *OPTICS EXPRESS*  
Andreasson, J., Martin, A. V., Liang, M., Timneanu, N., Aquila, A., Wang, F., Iwan, B., Svenda, M., Ekeberg, T., Hantke, M., Bielecki, J., Rolles, D., Rudenko, et al  
2014; 22 (3): 2497–2510
- **Imaging molecular structure through femtosecond photoelectron diffraction on aligned and oriented gas-phase molecules** *FARADAY DISCUSSIONS*  
Boll, R., Rouzee, A., Adolph, M., Anielski, D., Aquila, A., Bari, S., Bomme, C., Bostedt, C., Bozek, J. D., Chapman, H. N., Christensen, L., Coffee, R., Coppola, et al  
2014; 171: 57–80
- **Structure of a photosynthetic reaction centre determined by serial femtosecond crystallography** *NATURE COMMUNICATIONS*  
Johansson, L. C., Arnlund, D., Katona, G., White, T. A., Barty, A., DePonte, D. P., Shoeman, R. L., Wickstrand, C., Sharma, A., Williams, G. J., Aquila, A., Bogan, M. J., Caleman, et al  
2013; 4: 2911
- **Toward unsupervised single-shot diffractive imaging of heterogeneous particles using X-ray free-electron lasers** *OPTICS EXPRESS*  
Park, H. J., Loh, N. D., Sierra, R. G., Hampton, C. Y., Starodub, D., Martin, A. V., Barty, A., Aquila, A., Schulz, J., Steinbrener, J., Shoeman, R. L., Lomb, L., Kassemeyer, et al  
2013; 21 (23): 28729-28742
- **Mesoscale morphology of airborne core-shell nanoparticle clusters: x-ray laser coherent diffraction imaging** *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*  
Pedersoli, E., Loh, N. D., Capotondi, F., Hampton, C. Y., Sierra, R. G., Starodub, D., Bostedt, C., Bozek, J., Nelson, A. J., Aslam, M., Li, S., Dravid, V. P., Martin, et al  
2013; 46 (16)
- **Sensing the wavefront of x-ray free-electron lasers using aerosol spheres** *OPTICS EXPRESS*  
Loh, N. D., Starodub, D., Lomb, L., Hampton, C. Y., Martin, A. V., Sierra, R. G., Barty, A., Aquila, A., Schulz, J., Steinbrener, J., Shoeman, R. L., Kassemeyer, S., Bostedt, et al  
2013; 21 (10): 12385-12394
- **Natively Inhibited Trypanosoma brucei Cathepsin B Structure Determined by Using an X-ray Laser** *SCIENCE*  
Redecke, L., Nass, K., DePonte, D. P., White, T. A., Rehders, D., Barty, A., Stellato, F., Liang, M., Barends, T. M., Boutet, S., Williams, G. J., Messerschmidt, M., Seibert, et al  
2013; 339 (6116): 227–30
- **Results from single shot grazing incidence hard x-ray damage measurements conducted at the SACLA FEL**  
Aquila, A., Ozkan, C., Sobierajski, R., Hajkova, V., Burian, T., Chalupsky, J., Juha, L., Stoermer, M., Ohashi, H., Koyama, T., Tono, K., Inubushi, Y., Yabashi, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2013
- **Characterizing the focus of a multilayer coated off-axis parabola for FLASH beam at lambda=4.3 nm**  
Leontowich, A. G., Aquila, A., Stellato, F., Bean, R., Fleckenstein, H., Prasciolu, M., Liang, M., DePonte, D. P., Barty, A., Wang, F., Andreasson, J., Hajdu, J., Chapman, et al

SPIE-INT SOC OPTICAL ENGINEERING.2013

- **Single-particle structure determination by correlations of snapshot X-ray diffraction patterns** *NATURE COMMUNICATIONS*  
Starodub, D., Aquila, A., Bajt, S., Barthelmess, M., Barty, A., Bostedt, C., Bozek, J. D., Coppola, N., Doak, R. B., Epp, S. W., Erk, B., Foucar, L., GUMPRECHT, et al  
2012; 3
- **Ultra-efficient ionization of heavy atoms by intense X-ray free-electron laser pulses** *NATURE PHOTONICS*  
Rudek, B., Son, S., Foucar, L., Epp, S. W., Erk, B., Hartmann, R., Adolph, M., Andritschke, R., Aquila, A., Berrah, N., Bostedt, C., Bozek, J., Coppola, et al  
2012; 6 (12): 858-865
- **High-Resolution Protein Structure Determination by Serial Femtosecond Crystallography** *SCIENCE*  
Boutet, S., Lomb, L., Williams, G. J., Barends, T. R., Aquila, A., Doak, R. B., Weierstall, U., Deponte, D. P., Steinbrener, J., Shoeman, R. L., Messerschmidt, M., Barty, A., White, et al  
2012; 337 (6092): 362-364
- **Noise-robust coherent diffractive imaging with a single diffraction pattern** *OPTICS EXPRESS*  
Martin, A. V., Wang, F., Loh, N. D., Ekeberg, T., Maia, F. C., Hantke, M., van der Schot, G., Hampton, C. Y., Sierra, R. G., Aquila, A., Bajt, S., Barthelmess, M., Bostedt, et al  
2012; 20 (15): 16650–61
- **Fractal morphology, imaging and mass spectrometry of single aerosol particles in flight** *NATURE*  
Loh, N. D., Hampton, C. Y., Martin, A. V., Starodub, D., Sierra, R. G., Barty, A., Aquila, A., Schulz, J., Lomb, L., Steinbrener, J., Shoeman, R. L., Kassemeyer, S., Bostedt, et al  
2012; 486 (7404): 513-517
- **Nanoplasma Dynamics of Single Large Xenon Clusters Irradiated with Superintense X-Ray Pulses from the Linac Coherent Light Source Free-Electron Laser** *PHYSICAL REVIEW LETTERS*  
Gorkhover, T., Adolph, M., Rupp, D., Schorb, S., Epp, S. W., Erk, B., Foucar, L., Hartmann, R., Kimmel, N., Kuehnel, K., Rolles, D., Rudek, B., Rudenko, et al  
2012; 108 (24)
- **Femtosecond dark-field imaging with an X-ray free electron laser** *OPTICS EXPRESS*  
Martin, A. V., Loh, N. D., Hampton, C. Y., Sierra, R. G., Wang, F., Aquila, A., Bajt, S., Barthelmess, M., Bostedt, C., Bozek, J. D., Coppola, N., Epp, S. W., Erk, et al  
2012; 20 (12): 13501–12
- **CrystFEL: a software suite for snapshot serial crystallography** *JOURNAL OF APPLIED CRYSTALLOGRAPHY*  
White, T. A., Kirian, R. A., Martin, A. V., Aquila, A., Nass, K., Barty, A., Chapman, H. N.  
2012; 45: 335–41
- **In vivo protein crystallization opens new routes in structural biology** *NATURE METHODS*  
Koopmann, R., Cupelli, K., Redecke, L., Nass, K., Deponte, D. P., White, T. A., Stellato, F., Rehders, D., Liang, M., Andreasson, J., Aquila, A., Bajt, S., Barthelmess, et al  
2012; 9 (3): 259-U54
- **High-efficiency x-ray gratings with asymmetric-cut multilayers** *JOURNAL OF THE OPTICAL SOCIETY OF AMERICA A-OPTICS IMAGE SCIENCE AND VISION*  
Bajt, S., Chapman, H. N., Aquila, A., Gullikson, E.  
2012; 29 (3): 216–30
- **Lipidic phase membrane protein serial femtosecond crystallography** *NATURE METHODS*  
Johansson, L. C., Arnlund, D., White, T. A., Katona, G., Deponte, D. P., Weierstall, U., Doak, R. B., Shoeman, R. L., Lomb, L., Malmerberg, E., Davidsson, J., Nass, K., Liang, et al  
2012; 9 (3): 263-U59
- **Femtosecond free-electron laser x-ray diffraction data sets for algorithm development** *OPTICS EXPRESS*  
Kassemeyer, S., Steinbrener, J., Lomb, L., Hartmann, E., Aquila, A., Barty, A., Martin, A. V., Hampton, C. Y., Bajt, S., Barthelmess, M., Barends, T. R., Bostedt, C., Bott, et al  
2012; 20 (4): 4149-4158
- **Time-resolved protein nanocrystallography using an X-ray free-electron laser** *OPTICS EXPRESS*

- Aquila, A., Hunter, M. S., Doak, R., Kirian, R. A., Fromme, P., White, T. A., Andreasson, J., Arnlund, D., Bajt, S., Barends, T. M., Barthelmess, M., Bogan, M. J., Bostedt, et al  
2012; 20 (3): 2706–16
- **Self-terminating diffraction gates femtosecond X-ray nanocrystallography measurements.** *Nature photonics*  
Barty, A., Caleman, C., Aquila, A., Timneanu, N., Lomb, L., White, T. A., Andreasson, J., Arnlund, D., Bajt, S., Barends, T. R., Barthelmess, M., Bogan, M. J., Bostedt, et al  
2012; 6: 35-40
  - **In-band and out-of-band reflectance calibrations of the EUV multilayer mirrors of the Atmospheric Imaging Assembly instrument aboard the Solar Dynamics Observatory**  
Soufli, R., Spiller, E., Windt, D. L., Robinson, J. C., Gullikson, E. M., Rodriguez-de Marcos, L., Fernandez-Perea, M., Baker, S. L., Aquila, A. L., Dollar, F. J., Antonio Mendez, J., Larruquert, J. I., Golub, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2012
  - **Modeling of XFEL induced ionization and atomic displacement in protein nanocrystals**  
Caleman, C., Timneanu, N., Martin, A. V., White, T. A., Scott, H. A., Barty, A., Aquila, A., Chapman, H. N., Moeller, S. P., Yabashi, M., HauRiege, S. P.  
SPIE-INT SOC OPTICAL ENGINEERING.2012
  - **Profiling structured beams using injected aerosols** *Conference on X-Ray Free-Electron Lasers - Beam Diagnostics, Beamline Instrumentation, and Applications*  
Loh, N. D., Starodub, D., Lomb, L., Hampton, C. Y., Martin, A. V., Sierra, R. G., Barty, A., Aquila, A., Schulz, J., Steinbrener, J., Shoeman, R. L., Kassemeyer, S., Bostedt, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2012
  - **Self-terminating diffraction gates femtosecond X-ray nanocrystallography measurements** *NATURE PHOTONICS*  
Barty, A., Caleman, C., Aquila, A., Timneanu, N., Lomb, L., White, T. A., Andreasson, J., Arnlund, D., Bajt, S., Barends, T. R., Barthelmess, M., Bogan, M. J., Bostedt, et al  
2012; 6 (1): 35-40
  - **Multiphoton Ionization of Xenon at the LCLS Free-Electron Laser**  
Rudek, B., Rolles, D., Rudenko, A., Epp, S., Foucar, L., Erk, B., Hartmann, R., Kimmel, N., Holl, P., Reich, C., Strueder, L., Hirsemann, H., Ueda, et al  
IOP PUBLISHING LTD.2012
  - **Radiation damage in protein serial femtosecond crystallography using an x-ray free-electron laser** *PHYSICAL REVIEW B*  
Lomb, L., Barends, T. R., Kassemeyer, S., Aquila, A., Epp, S. W., Erk, B., Foucar, L., Hartmann, R., Rudek, B., Rolles, D., Rudenko, A., Shoeman, R. L., Andreasson, et al  
2011; 84 (21)
  - **Radiation damage in protein serial femtosecond crystallography using an x-ray free-electron laser.** *Physical review. B, Condensed matter and materials physics*  
Lomb, L., Barends, T. R., Kassemeyer, S., Aquila, A., Epp, S. W., Erk, B., Foucar, L., Hartmann, R., Rudek, B., Rolles, D., Rudenko, A., Shoeman, R. L., Andreasson, et al  
2011; 84 (21): 214111
  - **Unsupervised classification of single-particle X-ray diffraction snapshots by spectral clustering** *OPTICS EXPRESS*  
Yoon, C., Schwander, P., Abergel, C., Andersson, I., Andreasson, J., Aquila, A., Bajt, S., Barthelmess, M., Barty, A., Bogan, M. J., Bostedt, C., Bozek, J., Chapman, et al  
2011; 19 (17): 16542–49
  - **Structure-factor analysis of femtosecond micro-diffraction patterns from protein nanocrystals** *ACTA CRYSTALLOGRAPHICA SECTION A*  
Kirian, R. A., White, T. A., Holton, J. M., Chapman, H. N., Fromme, P., Barty, A., Lomb, L., Aquila, A., Maia, F. C., Martin, A. V., Fromme, R., Wang, X., Hunter, et al  
2011; 67: 131–40
  - **Femtosecond X-ray protein nanocrystallography** *NATURE*  
Chapman, H. N., Fromme, P., Barty, A., White, T. A., Kirian, R. A., Aquila, A., Hunter, M. S., Schulz, J., DePonte, D. P., Weierstall, U., Doak, R., Maia, F. C., Martin, et al  
2011; 470 (7332): 73–U81
  - **Single mimivirus particles intercepted and imaged with an X-ray laser** *NATURE*  
Seibert, M. M., Ekeberg, T., Maia, F. R., Svenda, M., Andreasson, J., Joensson, O., Odic, D., Iwan, B., Rucker, A., Westphal, D., Hantke, M., Deponte, D. P., Barty, et al



2011; 470 (7332): 78-U86

- **Polarization measurements of plasma excited X-ray lasers**  
Aquila, A., Bleiner, D., Balmer, J., Bajt, S., Dunn, J., Klisnick, A.  
SPIE-INT SOC OPTICAL ENGINEERING.2011
- **Single particle imaging with soft X-rays at the Linac Coherent Light Source** *Conference on Advances in X-ray Free-Electron Lasers - Radiation Schemes, X-ray Optics, and Instrumentation*  
Martin, A. V., Andreasson, J., Aquila, A., Bajt, S., Barends, T. R., Barthelmess, M., Barty, A., Benner, W. H., Bostedt, C., Bozek, J. D., Bucksbaum, P., Caleman, C., Coppola, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2011
- **Moving the Frontier of Quantum Control into the Soft X-Ray Spectrum** *INTERNATIONAL JOURNAL OF OPTICS*  
Aquila, A., Drescher, M., Laarmann, T., Barthelmess, M., Chapman, H. N., Bajt, S.  
2011
- **Optical constants of magnetron-sputtered magnesium films in the 25-1300 eV energy range** *JOURNAL OF APPLIED PHYSICS*  
Vidal-Dasilva, M., Aquila, A. L., Gullikson, E. M., Salmassi, F., Larruquert, J. I.  
2010; 108 (6)
- **Measuring the Structure of Epitaxially Assembled Block Copolymer Domains with Soft X-ray Diffraction** *MACROMOLECULES*  
Stein, G. E., Liddle, J., Aquila, A. L., Gullikson, E. M.  
2010; 43 (1): 433–41
- **Tri-material multilayer coatings with high reflectivity and wide bandwidth for 25 to 50 nm extreme ultraviolet light** *OPTICS EXPRESS*  
Aquila, A., Salmassi, F., Liu, Y., Gullikson, E. M.  
2009; 17 (24): 22102–7
- **Optical constants of evaporation-deposited silicon monoxide films in the 7.1-800 eV photon energy range** *JOURNAL OF APPLIED PHYSICS*  
Fernandez-Perea, M., Vidal-Dasilva, M., Larruquert, J. I., Aznarez, J. A., Mendez, J. A., Gullikson, E., Aquila, A., Soufli, R.  
2009; 105 (11)
- **Sub-micron focusing of a soft X-ray Free Electron Laser beam**  
Bajt, S., Chapman, H. N., Nelson, A. J., Lee, R. W., Toleikis, S., Mirkarimi, P., Alameda, J. B., Baker, S. L., Vollmer, H., Graff, R. T., Aquila, A., Gullikson, E. M., Ilse, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2009
- **Optical constants of magnetron-sputtered boron carbide thin films from photoabsorption data in the range 30 to 770 eV** *APPLIED OPTICS*  
Soufli, R., Aquila, A. L., Salmassi, F., Fernandez-Perea, M., Gullikson, E. M.  
2008; 47 (25): 4633–39
- **Absolute sensitivity calibration of extreme ultraviolet photoresists** *OPTICS EXPRESS*  
Naulleau, P. P., Gullikson, E. M., Aquila, A., George, S., Niakoula, D.  
2008; 16 (15): 11519–24
- **Single-cycle nonlinear optics** *SCIENCE*  
Goulielmakis, E., Schultze, M., Hofstetter, M., Yakovlev, V. S., Gagnon, J., Uiberacker, M., Aquila, A. L., Gullikson, E. M., Attwood, D. T., Kienberger, R., Krausz, F., Kleineberg, U.  
2008; 320 (5883): 1614–17
- **Metrologies for the phase characterization of attosecond extreme ultraviolet optics** *OPTICS LETTERS*  
Aquila, A., Salmassi, F., Gullikson, E.  
2008; 33 (5): 455–57
- **Development, characterization and experimental performance of x-ray optics for the LCLS free-electron laser**  
Soufli, R., Pivovarov, M. J., Baker, S. L., Robinson, J. C., Gullikson, E. M., McCarville, T. J., Stefan, P. M., Aquila, A. L., Ayers, J., McKernan, M. A., Bionta, R. M., Goto, S., Khounsary, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2008
- **Extreme ultraviolet resist outgassing and its effect on nearby optics**  
Denbeaux, G., Garg, R., Mbanaso, C., Waterman, J., Yankulin, L., Antohe, A., Fan, Y., Montgomery, W., Dean, K., Orvek, K., Wuest, A., Wei, Y., Goodwin, et al

SPIE-INT SOC OPTICAL ENGINEERING.2008

- **Optical constants of electron-beam evaporated boron films in the 6.8-900 eV photon energy range** *JOURNAL OF THE OPTICAL SOCIETY OF AMERICA A-OPTICS IMAGE SCIENCE AND VISION*  
Fernandez-Perea, M., Larruquert, J. I., Aznarez, J. A., Mendez, J. A., Vidal-Dasilva, M., Gullikson, E., Aquila, A., Soufli, R., Fierro, J. G.  
2007; 24 (12): 3800–3807
- **Multilayers for next generation x-ray sources**  
Bajt, S., Chapman, H. N., Spiller, E., Hau-Riege, S., Alameda, J., Nelson, A. J., Walton, C. C., Kjoernattawanich, B., Aquila, A., Dollar, F., Gullikson, E., Tarrío, C., Grantham, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2007
- **Developments in realistic design for aperiodic Mo/Si multilayer mirrors** *OPTICS EXPRESS*  
Aquila, A. L., Salmassi, F., Dollar, F., Liu, Y., Gullikson, M.  
2006; 14 (21): 10073–78
- **Oxidation resistance and microstructure of ruthenium-capped extreme ultraviolet lithography multilayers**  
Bajt, S., Dai, Z., Nelson, E. J., Wall, M. A., Alameda, J. B., Nguyen, N. Q., Baker, S. L., Robinson, J. C., Taylor, J. S., Aquila, A., Edwards, N.  
SPIE-INT SOCIETY OPTICAL ENGINEERING.2006
- **Oxidation resistance of Ru-capped EUV multilayers**  
Bajt, S., Dai, Z. R., Nelson, E. J., Wall, M. A., Alameda, J., Nguyen, N., Baker, S., Robinson, J. C., Taylor, J. S., Clift, M., Aquila, A., Gullikson, E. M., Edwards, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2005: 118–27
- **Substrate smoothing for high-temperature condenser operation in EUVL source environments**  
Soufli, R., Baker, S. L., Ratti, S., Robinson, J. C., Bajt, S. A., Alameda, J. B., Spiller, E., Taylor, J. S., Gullikson, E. M., Dollar, F. J., Aquila, A. L., Bristol, R. L., Mackay, et al  
SPIE-INT SOC OPTICAL ENGINEERING.2005: 140–45
- **Grating arrays for high-throughput soft X-ray spectrometers**  
Rasmussen, A., Aquila, A., Bookbinder, J., Chang, C., Gullikson, E., Heilmann, R. K., Kahn, S. M., Paerels, F., Schattenburg, M., Citterio, O., Odell, S. L.  
SPIE-INT SOC OPTICAL ENGINEERING.2004: 248–59
- **Iridium optical constants for the Chandra X-ray Observatory from reflectance measurements of 0.05-12 keV**  
Graessle, D. E., Soufli, R., Aquila, A. L., Gullikson, E. M., Blake, R. L., Burek, A. J., Flanagan, K. A., Siegmund, O. H.  
SPIE-INT SOC OPTICAL ENGINEERING.2004: 469–81
- **Measurements of the optical constants of scandium in the 50-1300eV range**  
Aquila, A. L., Salmassi, F., Gullikson, E. M., Eriksson, F., Birch, J., Soufli, R., Seely, J. F.  
SPIE-INT SOC OPTICAL ENGINEERING.2004: 64–71
- **Iridium optical constants from synchrotron reflectance measurements over 0.05-to 12-KeV x-ray energies**  
Graessle, D. E., Soufli, R., Nelson, A. J., Evans, C. L., Aquila, A. L., Gullikson, E. M., Blake, R. L., Burek, A. J., Soufli, R., Seely, J. F.  
SPIE-INT SOC OPTICAL ENGINEERING.2004: 72–83
- **Coherent soft x-ray generation in the water window with quasi-phase matching** *SCIENCE*  
Gibson, E. A., Paul, A., Wagner, N., Tobey, R., Gaudiosi, D., Backus, S., Christov, I. P., Aquila, A., Gullikson, E. M., Attwood, D. T., Murnane, M. M., Kapteyn, H. C.  
2003; 302 (5642): 95–98
- **Design and performance of capping layers for extreme-ultraviolet multilayer mirrors** *APPLIED OPTICS*  
Bajt, S. A., Chapman, H. N., Nguyen, N., Alameda, J., Robinson, J. C., Malinowski, M., Gullikson, E., Aquila, A., Tarrío, C., Grantham, S.  
2003; 42 (28): 5750–58
- **Comparison of extreme ultraviolet reflectance measurements** *JOURNAL OF MICROLITHOGRAPHY MICROFABRICATION AND MICROSYSTEMS*  
Scholze, F., Tummeler, J., Gullikson, E., Aquila, A.  
2003; 2 (3): 233–35