

## Andrew Lee Aquila

Staff Scientist, SLAC National Accelerator Laboratory

### Bio

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#### 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

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#### 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  
2024; 14 (1): 17283
- **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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2023; 94 (10)
- **Optical control of ultrafast structural dynamics in a fluorescent protein.** *Nature chemistry*  
Hutchison, C. D., Baxter, J. M., Fitzpatrick, A., Dorlhiac, G., Fadini, A., Perrett, S., Maghlaoui, K., Lefevre, S. B., Cordon-Preciado, V., Ferreira, J. L., Chukhutsina, V. U., Garratt, D., Barnard, et al  
2023
- **Regioselective, catalytic 1,1-difluorination of enynes** *NATURE CHEMISTRY*  
Wang, Z., Livingstone, K., Huempel, C., Daniliuc, C. G., Mueck-Lichtenfeld, C., Gilmour, R.  
2023; 15 (11): 1515-1522
- **Microstructure and crystal order during freezing of supercooled water drops.** *Nature*  
Kalita, A., Mrozek-McCourt, M., Kaldawi, T. F., Willmott, P. R., Loh, N. D., Marte, S., Sierra, R. G., Laksmono, H., Koglin, J. E., Hayes, M. J., Paul, R. H., Guillet, S. A., Aquila, et al

2023; 620 (7974): 557-561

- **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  
2023; 14 (1): 3384
- **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.  
2022; 106 (2)
- **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., Dahlgvist, 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., DeMirici, 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., Bolotovskiy, 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  
1800; 601 (7893): 360-365
- **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  
2021; 3 (1)
- **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*  
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  
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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., 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., Cojocar, 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  
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- **Evaluation of the performance of classification algorithms for XFEL single-particle imaging data** *IUCrJ*  
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- **Evaluation of the performance of classification algorithms for XFEL single-particle imaging data.** *IUCrJ*  
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- **The Macromolecular Femtosecond Crystallography Instrument at the Linac Coherent Light Source.** *Journal of synchrotron radiation*  
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- **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  
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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. 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., 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  
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*  
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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., 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.  
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  
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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  
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  - **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**  
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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**  
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  - **Protein structure determination by single-wavelength anomalous diffraction phasing of X-ray free-electron laser data IUCRJ**  
Nass, K., Meinhardt, 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  
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  - **Macromolecular diffractive imaging using imperfect crystals NATURE**  
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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  
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- **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  
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- **Concentric-flow electrokinetic injector enables serial crystallography of ribosome and photosystem II.** *Nature methods*  
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- **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.  
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- **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  
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- **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  
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- **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
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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  
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- **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  
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