Stanford

Thomas Wolf

Lead Scientist, SLAC National Accelerator Laboratory

Bio

BIO

Thomas Wolf is the head of the Chemical Sciences Department within the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory and a PI within the Stanford PULSE Institute. His research focuses on the investigation of photochemical dynamics in isolated organic molecules with novel experimental tools such as ultrashort X-ray and electron pulses. Thomas received his master's degree in Chemistry from University of Karlsruhe, Germany, in 2009. In 2012, he finished his PhD degree in Physical Chemistry at Karlsruhe Institute of Technology, Germany. After a postdoctoral stay at Karlsruhe Institute of Technology, he joined the Gühr research group as a postdoc at SLAC National Accelerator Laboratory in 2013. He has been working as a PI within the Stanford PULSE Institute since 2016 and since 2021 in the role as Chemical Sciences Department head at LCLS.

CURRENT ROLE AT STANFORD

Chemical Science Department Head, Linac Coherent Light Source (LCLS)

Principal Investigator, Stanford PULSE Institute, SLAC National Accelerator Laboratory

INSTITUTE AFFILIATIONS

- Principal Investigator, Stanford PULSE Institute

EDUCATION AND CERTIFICATIONS

- Dipl. Chem., Karlsruhe University , Chemistry (2009)
- Dr. rer. nat., Karlsruhe Institute of Technology , Physical Chemistry (2012)

LINKS

- Group website: http://www.wolfresearchgroup.com/
- LCLS Chemical Sciences Department website: https://lcls.slac.stanford.edu/depts/chemsci
- Stanford PULSE Institute: https://ultrafast.stanford.edu/

Professional

PROFESSIONAL INTERESTS

I am interested in ultrafast photoinduced dynamics of organic molecules. Ultrafast photoinduced dynamics involve correlated electronic and nuclear motion in the vicinity of conical intersections between different electronic states. To understand in detail, what drives a molecule like cyclohexadiene to undergo an electrocyclic reaction within less than 100 femtoseconds after absorption of an ultraviolet photon or a nucleobase like thymine to instead dissipate the absorbed energy into heat on the same timescale, direct access to the electronic and nuclear dynamics on the timescale of

those processes is required. To achieve this, I combine femtosecond time-resolved gas phase VUV and soft x-ray spectroscopy to investigate ultrafast changes in the electronic structure with electron diffraction to obtain exclusive access to the correlated dynamics of the nuclear wavepacket.

PROFESSIONAL AFFILIATIONS AND ACTIVITIES

- Chemical Science Department Head, Linac Coherent Light Source (2021 - present)
- Principal Investigator of the Excited States in Isolate Molecules group, Stanford PULSE Institute (2016 - present)

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
- **Ultrafast x-ray scattering of photodissociation dynamics in 2-iodothiophene.** *The Journal of chemical physics*
  Razmus, W. O., Gabalski, I., Allum, F., Abma, G. L., Britton, M., Boutet, S., Bucksbaum, P. H., Cheng, X., Crane, S. W., Gate, G., Ghrist, A., Graßl, M., Green, et al
  2026; 164 (2)
- **The UV Photoinduced Ring-Closing Reaction of Cyclopentadiene Probed with Ultrafast Electron Diffraction.** *The journal of physical chemistry. A*
  Lederer, J., Bertram, L., Huang, L., Bhattacharyya, S., Boutet, S., Cheng, X., Crane, S. W., England, R. J., Graßl, M., Heald, L., Ji, F., Kramer, P., Lam, et al
  2025
- **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., Glownia, J., Gong, X., Hammerland, D., Han, M., Heck, et al
  2025; 15 (4)
- **Investigating the ultraviolet photodissociation of bromocyclopropane with ultrafast electron diffraction.** *The Journal of chemical physics*
  Lederer, J., Nunes, J. P., Rankine, C. D., Attar, A. R., Hegazy, K., Ji, F., Le, C., Lin, M. F., Liu, Y., Luo, D., Orr-Ewing, A. J., Saha, S. K., Shen, et al
  2025; 163 (17)
- **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
- **Structural dynamics of laser-ionized cis-stilbene studied by ultrafast electron diffraction** *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*
  Saha, S. K., Nunes, J. P. F., Weir, H., Moore, B., Williams, M., Attar, A. R., Luo, D., Ji, F., Heald, L., Hoffmann, M. C., Yang, J., Lin, M., Ware, et al
  2025; 58 (17)
- **Imaging Valence Electron Rearrangement in a Chemical Reaction Using Hard X-Ray Scattering.** *Physical review letters*
  Gabalski, I., Green, A., Lenzen, P., Allum, F., Bain, M., Bhattacharyya, S., Britton, M. A., Champenois, E. G., Cheng, X., Cryan, J. P., Driver, T., Forbes, R., Garratt, et al
  2025; 135 (8): 083001
- **Imaging Valence Electron Rearrangement in a Chemical Reaction Using Hard X-Ray Scattering** *PHYSICAL REVIEW LETTERS*
  Gabalski, I., Green, A., Lenzen, P., Allum, F., Bain, M., Bhattacharyya, S., Britton, M. A., Champenois, E. G., Cheng, X., Cryan, J. P., Driver, T., Forbes, R., Garratt, et al
  2025; 135 (8)
- **Real-space observation of the dissociation of a transition metal complex and its concurrent energy redistribution.** *Nature communications*
  Schori, A., Biasin, E., Banerjee, A., Boutet, S., Bucksbaum, P. H., Carbajo, S., Gaffney, K. J., Glownia, J. M., Hartsock, R., Ledbetter, K., Kaldun, A., Koglin, J. E., Kunnus, et al
  2025; 16 (1): 4767

- **Capturing Ring Opening in Photoexcited Enolic Acetylacetone upon Hydrogen Bond Dissociation by Ultrafast Electron Diffraction.** *The journal of physical chemistry letters*
  Scutelnic, V., Tikhonov, D. S., Marggi Poullain, S., Haugen, E. A., Attar, A., Barreau, L., Chang, K., Fidler, A. P., Gaynor, J. D., Lin, Y., Yang, J., Champenois, E. G., Wang, et al
  2025: 5068-5075

- **Direct Observation of the ππ* to nπ* Transition in 2-Thiouracil via Time-Resolved NEXAFS Spectroscopy.** *The journal of physical chemistry letters*
  Lever, F., Picconi, D., Mayer, D., Ališauskas, S., Calegari, F., Düsterer, S., Feifel, R., Kuhlmann, M., Mazza, T., Metje, J., Robinson, M. S., Squibb, R. J., Trabattoni, et al
  2025: 4038-4046

- **Ultrafast Events in Electrocyclic Ring-Opening Reactions.** *Annual review of physical chemistry*
  Liu, Y., Xu, R., Sanchez, D. M., Martínez, T. J., Wolf, T. J.
  2025

- **Probing Electronic Coherence between Core-Level Vacancies at Different Atomic Sites** *PHYSICAL REVIEW X*
  Wang, J., Driver, T.
  2025; 15: 011008

- **Ultrafast structural dynamics of UV photoexcited cis,cis-1,3-cyclooctadiene observed with time-resolved electron diffraction.** *Physical chemistry chemical physics : PCCP*
  Muvva, S. B., Liu, Y., Chakraborty, P., Nunes, J. P., Attar, A. R., Bhattacharyya, S., Borne, K., Champenois, E. G., Goff, N., Hegazy, K., Hoffmann, M. C., Ji, F., Lin, et al
  2024

- **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)

- **Photoinduced hydrogen dissociation in thymine predicted by coupled cluster theory.** *Nature communications*
  Kjønstad, E. F., Fajen, O. J., Paul, A. C., Angelico, S., Mayer, D., Gühr, M., Wolf, T. J., Martínez, T. J., Koch, H.
  2024; 15 (1): 10128

- **Quantitative x-ray scattering of free molecules** *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*
  Ma, L., Goff, N., Carrascosa, A., Nelson, S., Liang, M., Cheng, X., Yong, H., Gabalski, I., Huang, L., Crane, S. W., Green, A. E., Allum, F., Lenzen, et al
  2024; 57 (20)

- **Tracking dissociation pathways of nitrobenzene via mega-electron-volt ultrafast electron diffraction** *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*
  Hegazy, K., Bucksbaum, P., Centurion, M., Cryan, J., Li, R., Lin, M., Moore, B., Nunes, P., Shen, X., Weathersby, S., Yang, J., Wang, X., Wolf, et al
  2024; 57 (19)

- **UV-Induced Reaction Pathways in Bromoform Probed with Ultrafast Electron Diffraction.** *Journal of the American Chemical Society*
  Hoffmann, L., Toulson, B. W., Yang, J., Saladrigas, C. A., Zong, A., Muvva, S. B., Figueira Nunes, J. P., Reid, A. H., Attar, A. R., Luo, D., Ji, F., Lin, M. F., Fan, et al
  2024

- **Attosecond delays in X-ray molecular ionization.** *Nature*
  Driver, T., Mountney, M., Wang, J., Ortmann, L., Al-Haddad, A., Berrah, N., Bostedt, C., Champenois, E. G., DiMauro, L. F., Duris, J., Garratt, D., Glownia, J. M., Guo, et al
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- **The Ring-Closing Reaction of Cyclopentadiene Probed with Ultrafast X-ray Scattering.** *The journal of physical chemistry. A*
  Huang, L., Bertram, L., Ma, L., Goff, N., Crane, S. W., Odate, A., Northey, T., Carrascosa, A. M., Simmermacher, M., Muvva, S. B., Geiser, J. D., Lueckheide, M. J., Phelps, et al
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- **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
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- **Monitoring the Evolution of Relative Product Populations at Early Times during a Photochemical Reaction.** *Journal of the American Chemical Society*
  Figueira Nunes, J. P., Ibele, L. M., Pathak, S., Attar, A. R., Bhattacharyya, S., Boll, R., Borne, K., Centurion, M., Erk, B., Lin, M., Forbes, R. J., Goff, N., Hansen, et al
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- **Compact single-shot soft X-ray photon spectrometer for free-electron laser diagnostics** *OPTICS EXPRESS*
  Larsen, K. A., Borne, K., Obaid, R., Kamalov, A., Liu, Y., Cheng, X., James, J., Driver, T., Li, K., Liu, Y., Sakdinawat, A., David, C., Wolf, et al
  2023; 31 (22): 35822-35834

- **Femtosecond Electronic and Hydrogen Structural Dynamics in Ammonia Imaged with Ultrafast Electron Diffraction.** *Physical review letters*
  Champenois, E. G., List, N. H., Ware, M., Britton, M., Bucksbaum, P. H., Cheng, X., Centurion, M., Cryan, J. P., Forbes, R., Gabalski, I., Hegazy, K., Hoffmann, M. C., Howard, et al
  2023; 131 (14): 143001

- **Transient vibration and product formation of photoexcited CS2 measured by time-resolved x-ray scattering.** *The Journal of chemical physics*
  Gabalski, I., Sere, M., Acheson, K., Allum, F., Boutet, S., Dixit, G., Forbes, R., Glownia, J. M., Goff, N., Hegazy, K., Howard, A. J., Liang, M., Minitti, et al
  2022; 157 (16): 164305

- **The time-resolved atomic, molecular and optical science instrument at the Linac Coherent Light Source.** *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
  2022; 29 (Pt 4): 957-968

- **Multichannel photodissociation dynamics in CS2 studied by ultrafast electron diffraction.** *Physical chemistry chemical physics : PCCP*
  Razmus, W. O., Acheson, K., Bucksbaum, P., Centurion, M., Champenois, E., Gabalski, I., Hoffman, M. C., Howard, A., Lin, M., Liu, Y., Nunes, P., Saha, S., Shen, et al
  2022

- **Attosecond coherent electron motion in Auger-Meitner decay.** *Science (New York, N.Y.)*
  Li, S., Driver, T., Rosenberger, P., Champenois, E. G., Duris, J., Al-Haddad, A., Averbukh, V., Barnard, J. C., Berrah, N., Bostedt, C., Bucksbaum, P. H., Coffee, R. N., DiMauro, et al
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- **Ultrafast Imaging of Molecules with Electron Diffraction.** *Annual review of physical chemistry*
  Centurion, M., Wolf, T. J., Yang, J.
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- **Core-Level Spectroscopy of 2-Thiouracil at the Sulfur L1- and L2,3-Edges Utilizing a SASE Free-Electron Laser.** *Molecules (Basel, Switzerland)*
  Lever, F., Mayer, D., Metje, J., Alisauskas, S., Calegari, F., Dusterer, S., Feifel, R., Niebuhr, M., Manschwetus, B., Kuhlmann, M., Mazza, T., Robinson, M. S., Squibb, et al
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- **Site-specific interrogation of an ionic chiral fragment during photolysis using an X-ray free-electron laser** *COMMUNICATIONS CHEMISTRY*
  Ilchen, M., Schmidt, P., Novikovskiy, N. M., Hartmann, G., Rupprecht, P., Coffee, R. N., Ehresmann, A., Galler, A., Hartmann, N., Helml, W., Huang, Z., Inhester, L., Lutman, et al
  2021; 4 (1)

- **Site-specific interrogation of an ionic chiral fragment during photolysis using an X-ray free-electron laser.** *Communications chemistry*
  Ilchen, M., Schmidt, P., Novikovskiy, N. M., Hartmann, G., Rupprecht, P., Coffee, R. N., Ehresmann, A., Galler, A., Hartmann, N., Helml, W., Huang, Z., Inhester, L., Lutman, et al
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- **Direct observation of ultrafast hydrogen bond strengthening in liquid water.** *Nature*

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- **Transient resonant Auger-Meitner spectra of photoexcited thymine.** *Faraday discussions*

  Wolf, T. J., Paul, A. C., Folkestad, S. D., Myhre, R. H., Cryan, J. P., Berrah, N., Bucksbaum, P. H., Coriani, S., Coslovich, G., Feifel, R., Martinez, T. J., Moeller, S. P., Mucke, et al

  2021

- **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

- **Conformer-specific photochemistry imaged in real space and time.** *Science (New York, N.Y.)*

  Champenois, E. G., Sanchez, D. M., Yang, J., Figueira Nunes, J. P., Attar, A., Centurion, M., Forbes, R., Gühr, M., Hegazy, K., Ji, F., Saha, S. K., Liu, Y., Lin, et al

  2021; 374 (6564): 178-182

- **Arrival Time Monitor for Sub-10 fs Soft X-ray and 800 nm Optical Pulses**

  Muhammad, I., Frimpong, B., Daafour, J., Xu, X., Walter, P., Wolf, T. J. A., Cryan, J. P., Glownia, J. M., Robinson, J. S., Droste, S., Coslovich, G., IEEE

  IEEE.2021

- **Structure retrieval in liquid-phase electron scattering.** *Physical chemistry chemical physics : PCCP*

  Yang, J., Nunes, J. P., Ledbetter, K., Biasin, E., Centurion, M., Chen, Z., Cordones, A. A., Crissman, C., Deponte, D. P., Glenzer, S. H., Lin, M., Mo, M., Rankine, et al

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- **Spectroscopic and Structural Probing of Excited-State Molecular Dynamics with Time-Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction** *PHYSICAL REVIEW X*

  Liu, Y., Horton, S. L., Yang, J., Nunes, J. F., Shen, X., Wolfe, T. J. A., Forbes, R., Cheng, C., Moore, B., Centurion, M., Hegazy, K., Li, R., Lin, et al

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- **Liquid-phase mega-electron-volt ultrafast electron diffraction** *STRUCTURAL DYNAMICS-US*

  Nunes, J. F., Ledbetter, K., Lin, M., Kozina, M., DePonte, D. P., Biasin, E., Centurion, M., Crissman, C. J., Dunning, M., Guillet, S., Jobe, K., Liu, Y., Mo, et al

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- **Simultaneous observation of nuclear and electronic dynamics by ultrafast electron diffraction.** *Science (New York, N.Y.)*

  Yang, J. n., Zhu, X. n., F Nunes, J. P., Yu, J. K., Parrish, R. M., Wolf, T. J., Centurion, M. n., Gühr, M. n., Li, R. n., Liu, Y. n., Moore, B. n., Niebuhr, M. n., Park, et al

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- **Tunable isolated attosecond X-ray pulses with gigawatt peak power from a free-electron laser** *NATURE PHOTONICS*

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  Driver, T., Li, S., Champenois, E. G., Duris, J., Ratner, D., Lane, T. J., Rosenberger, P., Al-Haddad, A., Averbukh, V., Barnard, T., Berrah, N., Bostedt, C., Bucksbaum, et al

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- **Spectroscopic Signature of Chemical Bond Dissociation Revealed by Calculated Core-Electron Spectra.** *The journal of physical chemistry letters*
  Inhester, L., Li, Z., Zhu, X., Medvedev, N., Wolf, T. J.
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- **Femtosecond gas-phase mega-electron-volt ultrafast electron diffraction.** *Structural dynamics (Melville, N.Y.)*
  Shen, X., Nunes, J. P., Yang, J., Jobe, R. K., Li, R. K., Lin, M., Moore, B., Niebuhr, M., Weathersby, S. P., Wolf, T. J., Yoneda, C., Guehr, M., Centurion, et al
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  Wolf, T. A., Sanchez, D. M., Yang, J., Parrish, R. M., Nunes, J. F., Centurion, M., Coffee, R., Cryan, J. P., Guehr, M., Hegazy, K., Kirrander, A., Li, R. K., Ruddock, et al
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- **Observation of Ultrafast Intersystem Crossing in Thymine by Extreme Ultraviolet Time-Resolved Photoelectron Spectroscopy.** *The journal of physical chemistry. A*
  Wolf, T. J., Parrish, R. M., Myhre, R. H., Martínez, T. J., Koch, H. n., Gühr, M. n.
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- **Photo-ionization and fragmentation of Sc3N@C80 following excitation above the Sc K-edge.** *The Journal of chemical physics*
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  Battistoni, A., Durr, H. A., Guehr, M., Wolf, T. A.
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- **Normal and resonant Auger spectroscopy of isocyanic acid, HNCO** *JOURNAL OF CHEMICAL PHYSICS*
  Holzmeier, F., Wolf, T. A., Gienger, C., Wagner, Bozek, J., Nandi, S., Nicolas, C., Fischer, Guehr, M., Fink, R. F.
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  Xiong, H., Fang, L., Osipov, T., Kling, N. G., Wolf, T. J. A., Sistrunk, E., Obaid, R., Guehr, M., Berrah, N.
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- **A theoretical and experimental benchmark study of core-excited states in nitrogen** *JOURNAL OF CHEMICAL PHYSICS*
  Myhre, R. H., Wolf, T. J. A., Cheng, L., Nandi, S., Coriani, S., Guhr, M., Koch, H.
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- **Time-resolved photoelectron spectroscopy of nitrobenzene and its aldehydes** *CHEMICAL PHYSICS LETTERS*
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- **Soft-x-ray-induced ionization and fragmentation dynamics of Sc3N@C-80 investigated using an ion-ion-coincidence momentum-imaging technique** *PHYSICAL REVIEW A*
  Xiong, H., Obaid, R., Fang, L., Bomme, C., Kling, N. G., Ablikim, U., Petrovic, V., Liekhus-Schmaltz, C. E., Li, H., Bilodeau, R. C., Wolf, T., Osipov, T., Rolles, et al
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  Ilchen, M., Hartmann, G., Rupprecht, P., Artemyev, A. N., Coffee, R. N., Li, Z., Ohldag, H., Ogasawara, H., Osipov, T., Ray, D., Schmidt, P., Wolf, T. A., Ehresmann, et al
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