

Stanford



Thomas Wolf

Staff Scientist, SLAC National Accelerator Laboratory

Bio

BIO

I am a Staff Scientist at SLAC National Accelerator Laboratory. I received my master's degree in Chemistry from University of Karlsruhe, Germany, in 2009. In 2012, I finished my PhD degree in Physical Chemistry at Karlsruhe Institute of Technology, Germany. After a postdoctoral stay at Karlsruhe Institute of Technology, I joined the Gühr research group at SLAC National Accelerator Laboratory in 2013. I have been working in my current role as PI of the Excited States in Isolated Molecules group within the Stanford PULSE Institute since 2016.

EDUCATION AND CERTIFICATIONS

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

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

- Principal Investigator of the Excited States in Isolate Molecules group, Stanford PULSE Institute (2016 - present)

Publications

PUBLICATIONS

- **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*
Yang, J., Dettori, R., Nunes, J. P., List, N. H., Biasin, E., Centurion, M., Chen, Z., Cordones, A. A., Deponte, D. P., Heinz, T. F., Kozina, M. E., Ledbetter, K., Lin, et al

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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
- **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
2020
- **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. A., Forbes, R., Cheng, C., Moore, B., Centurion, M., Hegazy, K., Li, R., Lin, et al
2020; 10 (2)
- **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
2020; 7 (2): 024301
- **Intermolecular Coulombic Decay in Endohedral Fullerene at the 4d#4f Resonance.** *Physical review letters*
Obaid, R. n., Xiong, H. n., Augustin, S. n., Schnorr, K. n., Ablikim, U. n., Battistoni, A. n., Wolf, T. J., Bilodeau, R. C., Osipov, T. n., Gokhberg, K. n., Rolles, D. n., LaForge, A. C., Berrah, et al
2020; 124 (11): 113002
- **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
2020; 368 (6493): 885–89
- **Tunable isolated attosecond X-ray pulses with gigawatt peak power from a free-electron laser** *NATURE PHOTONICS*
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- **Attosecond transient absorption spooktroscopy: a ghost imaging approach to ultrafast absorption spectroscopy.** *Physical chemistry chemical physics : PCCP*
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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- **Femtosecond-resolved observation of the fragmentation of buckminsterfullerene following X-ray multiphoton ionization** *NATURE PHYSICS*
Berrah, N., Sanchez-Gonzalez, A., Jurek, Z., Obaid, R., Xiong, H., Squibb, R. J., Osipov, T., Lutman, A., Fang, L., Barillot, T., Bozek, J. D., Cryan, J., Wolf, et al
2019; 15 (12): 1279–+
- **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.
2019; 6536–44
- **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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- **Diffraction imaging of dissociation and ground-state dynamics in a complex molecule** *PHYSICAL REVIEW A*
Wilkin, K. J., Parrish, R. M., Yang, J., Wolf, T. A., Nunes, J. F., Guehr, M., Li, R., Shen, X., Zheng, Q., Wang, X., Martinez, T. J., Centurion, M.
2019; 100 (2)

- **The photochemical ring-opening of 1,3-cyclohexadiene imaged by ultrafast electron diffraction** *NATURE CHEMISTRY*
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
2019; 11 (6): 504–9
- **Photochemical pathways in nucleobases measured with an X-ray FEL.** *Philosophical transactions. Series A, Mathematical, physical, and engineering sciences*
Wolf, T. J., Guhr, M.
2019; 377 (2145): 20170473
- **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.
2019
- **Photo-ionization and fragmentation of Sc3N@C80 following excitation above the Sc K-edge.** *The Journal of chemical physics*
Obaid, R. n., Schnorr, K. n., Wolf, T. J., Takanashi, T. n., Kling, N. G., Kooser, K. n., Nagaya, K. n., Wada, S. I., Fang, L. n., Augustin, S. n., You, D. n., Campbell, E. E., Fukuzawa, et al
2019; 151 (10): 104308
- **Generation and Characterization of Attosecond Pulses from an X-ray Free-electron Laser**
Li, S., Rosenberger, P., Champenois, E. G., Driver, T., Bucksbaum, P. H., Coffee, R., Gattton, A., Hartmann, G., Helml, W., Huang, Z., Knurr, J., Kling, M. F., Lin, et al
IEEE.2019
- **A tilted pulse-front setup for femtosecond transient grating spectroscopy in highly non-collinear geometries** *JOURNAL OF OPTICS*
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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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- **Fragmentation of endohedral fullerene Ho3N@C-80 in an intense femtosecond near-infrared laser field** *PHYSICAL REVIEW A*
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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. 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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- **Imaging CF3I conical intersection and photodissociation dynamics with ultrafast electron diffraction** *Science*
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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*
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- **Observing Femtosecond Fragmentation Using Ultrafast X-ray-Induced Auger Spectra** *APPLIED SCIENCES-BASEL*
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2017; 7 (7)
- **Probing ultrafast pi pi*/n pi* internal conversion in organic chromophores via K-edge resonant absorption** *NATURE COMMUNICATIONS*

- Wolf, T. A., Myhre, R. H., Cryan, J. P., Coriani, S., Squibb, R. J., Battistoni, A., Berrah, N., Bostedt, C., Bucksbaum, P., Coslovich, G., Feifel, R., Gaffney, K. J., Grilj, et al
2017; 8: 29
- **Emitter-site-selective photoelectron circular dichroism of trifluoromethyloxirane** *PHYSICAL REVIEW A*
Ichen, 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
2017; 95 (5)
 - **The Role of Super-Atom Molecular Orbitals in Doped Fullerenes in a Femtosecond Intense Laser Field** *SCIENTIFIC REPORTS*
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 - **Gas Phase Photochemistry Probed by Free Electron Lasers** *X-Ray Free Electron Lasers: Applications in Materials, Chemistry and Biology*
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Royal Society of Chemistry.2017; 1: 173–186
 - **Auger electron and photoabsorption spectra of glycine in the vicinity of the oxygen K-edge measured with an X-FEL** *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*
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 - **Ultrafast Dynamics of o-Nitrophenol: An Experimental and Theoretical Study** *JOURNAL OF PHYSICAL CHEMISTRY A*
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 - **Time-Resolved Photoelectron Spectroscopy and Ab Initio Multiple Spawning Studies of Hexamethylcyclopentadiene**
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 - **Femtosecond photoelectron and photoion spectrometer with vacuum ultraviolet probe pulses** *JOURNAL OF ELECTRON SPECTROSCOPY AND RELATED PHENOMENA*
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Frick, E., Ernst, H. A., Voll, D., Wolf, T. J., Unterreiner, A., Barner-Kowollik, C.
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 - **Hexamethylcyclopentadiene: time-resolved photoelectron spectroscopy and ab initio multiple spawning simulations.** *Physical chemistry chemical physics*
Wolf, T. J., Kuhlman, T. S., Schalk, O., Martínez, T. J., Møller, K. B., Stolow, A., Unterreiner, A.
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 - **Synthesis and Application of Photolithographically Patternable Deep Blue Emitting Poly(3,6-Dimethoxy-9,9-dialkylsilafuorene)s** *ACS APPLIED MATERIALS & INTERFACES*
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 - **Three-dimensional multi-photon direct laser writing with variable repetition rate** *OPTICS EXPRESS*
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- **Electron tunneling from electronically excited states of isolated bisdisulizole-derived trianion chromophores following UV absorption** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
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E D P SCIENCES.2013
- **Ultrafast photoinduced dynamics of halogenated cyclopentadienes: observation of geminate charge-transfer complexes in solution** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
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- **Resonant tunneling through the repulsive Coulomb barrier of a quadruply charged molecular anion** *PHYSICAL REVIEW A*
Phuong Diem Dau, P. D., Liu, H., Yang, J., Winghart, M., Wolf, T. J., Unterreiner, A., Weis, P., Miao, Y., Ning, C., Kappes, M. M., Wang, L.
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