Science enabled by the high-brightness electron beams

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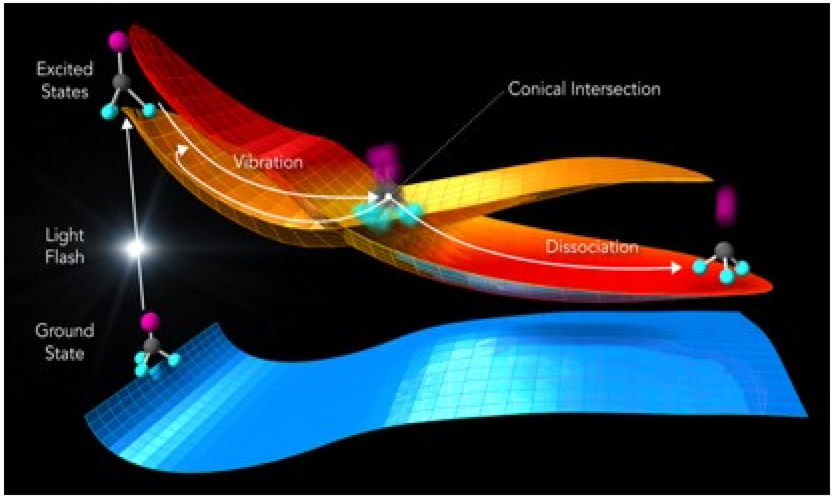
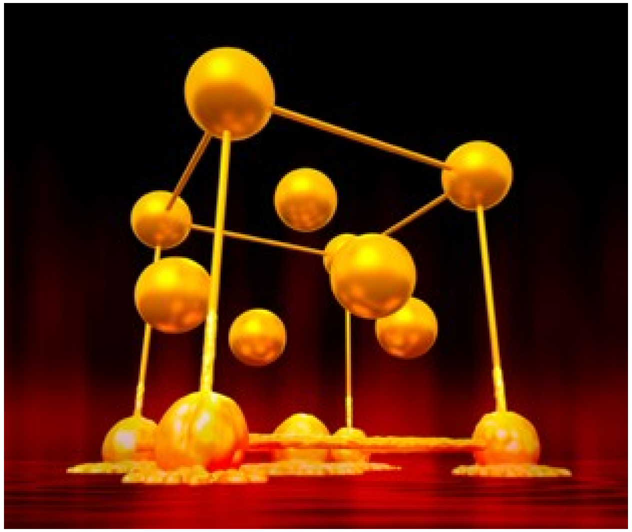
Physics Colloquium in Zeuthen
August 28, 2019

Science enabled by the high-brightness electron beams

Science enabled by the high-brightness MeV electron beams



Bond-breaking & nuclear wavepacket passing through conical intersections (*Science 361 64–67 (2018)*)



Resolving ultrafast phase transitions (*Science 360 1451–1455 (2018)*)

CHEMICAL PHYSICS

Imaging CF_3I conical intersection and photodissociation dynamics with ultrafast electron diffraction

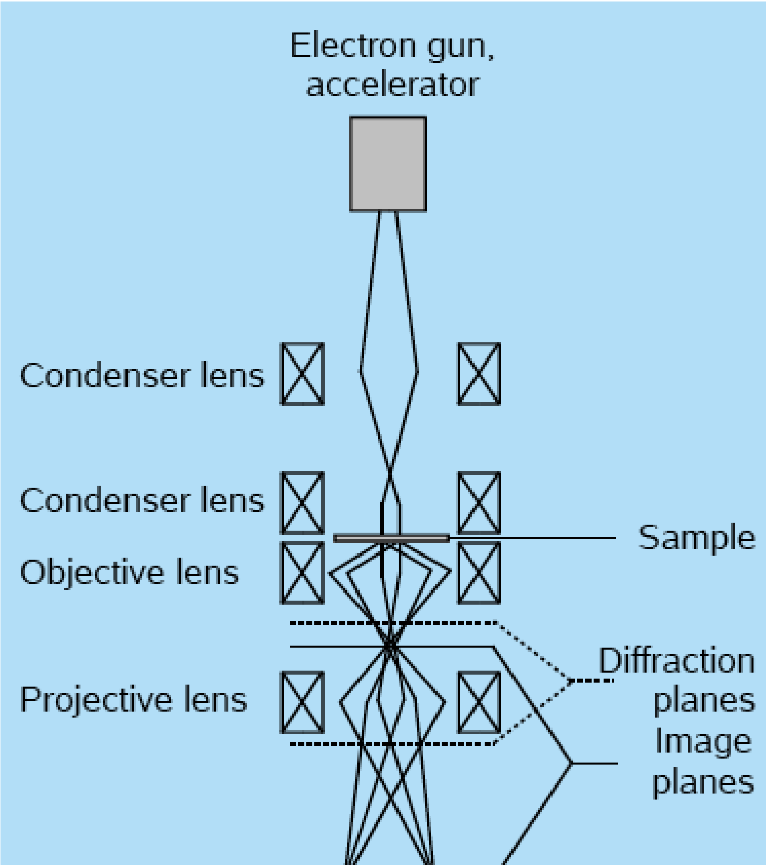
Jie Yang[1,2*], Xiaolei Zhu[2,3], Thomas J. A. Wolf[2], Zheng Li[2,4,5], J. Pedro F. Nunes[6], Ryan Coffee[2,7,8], James P. Cryan[2], Markus Gühr[2,9], Kareem Hegazy[2,8], Tony F. Heinz[2,10], Keith Jobe[1], Renkai Li[1], Xiaozhe Shen[1], Theodore Veccione[1], Stephen Weathersby[1], Kyle J. Wilkin[11], Charles Yoneda[1], Qiang Zheng[1], Todd J. Martinez[2,3*], Martin Centurion[11*], Xijie Wang[1*]

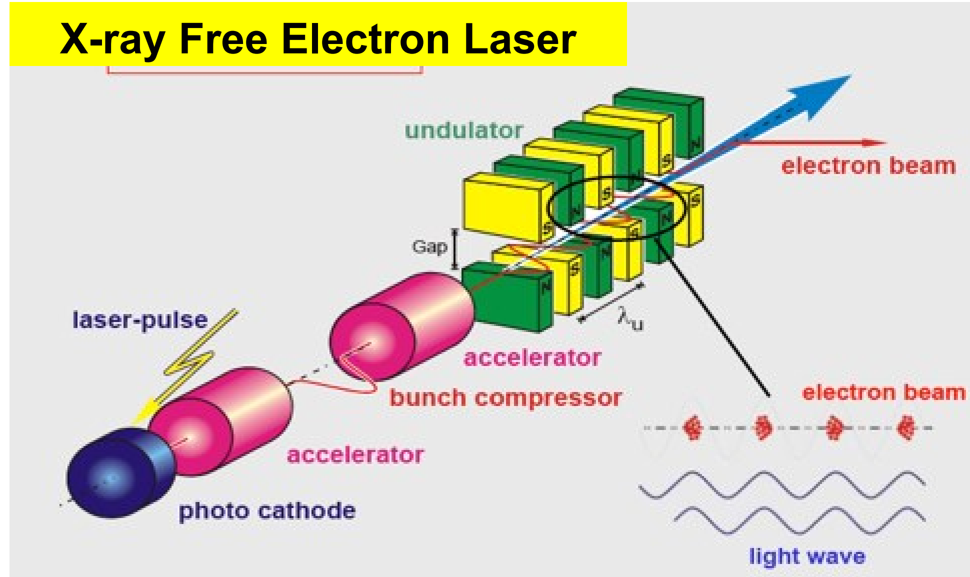
CONDENSED MATTER

Heterogeneous to homogeneous melting transition visualized with ultrafast electron diffraction

M. Z. Mo[1*†], Z. Chen[1†], R. K. Li[1], M. Dunning[1], B. B. L. Witte[1,2], J. K. Baldwin[3], L. B. Fletcher[1], J. B. Kim[1], A. Ng[4], R. Redmer[2], A. H. Reid[1], P. Shekhar[5], X. Z. Shen[1], M. Shen[5], K. Sokolowski-Tinten[6], Y. Y. Tsui[5], Y. Q. Wang[3], Q. Zheng[1], X. J. Wang[1], S. H. Glenzer[1*]

Brighter e⁻ Source → Better X-ray & Electron Instruments





Electron source

$$\lambda_{\min}[\mathrm{A}] = 4\frac{\pi\varepsilon_n[mm-mrad]}{\sqrt{I[kA]L_w[m]}}$$

Source Brightness

Contrast and Pixel Count

Time Resolution

$$\text{Brightness } B = \frac{Ne}{(\pi r^2)(\pi\alpha^2)\Delta t}$$

Spatial Resolution

Spatial Coherence

Photo Electron Source

Melting of Thin-Film Al (20 ps)

Mourou *et al.*, Appl. Phys. Lett. **41**, 44 (1982)

Williamson *et al.*, Phys. Rev. Lett. **52**, 2364 (1984)

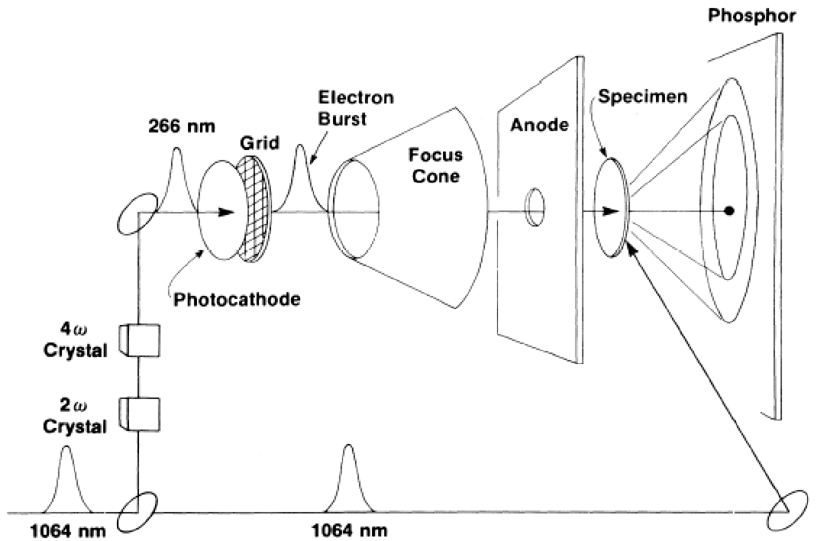
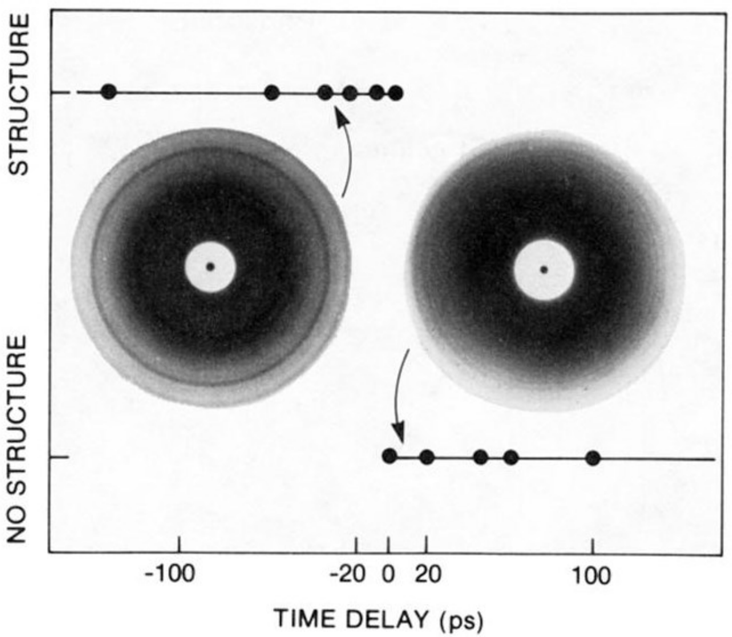
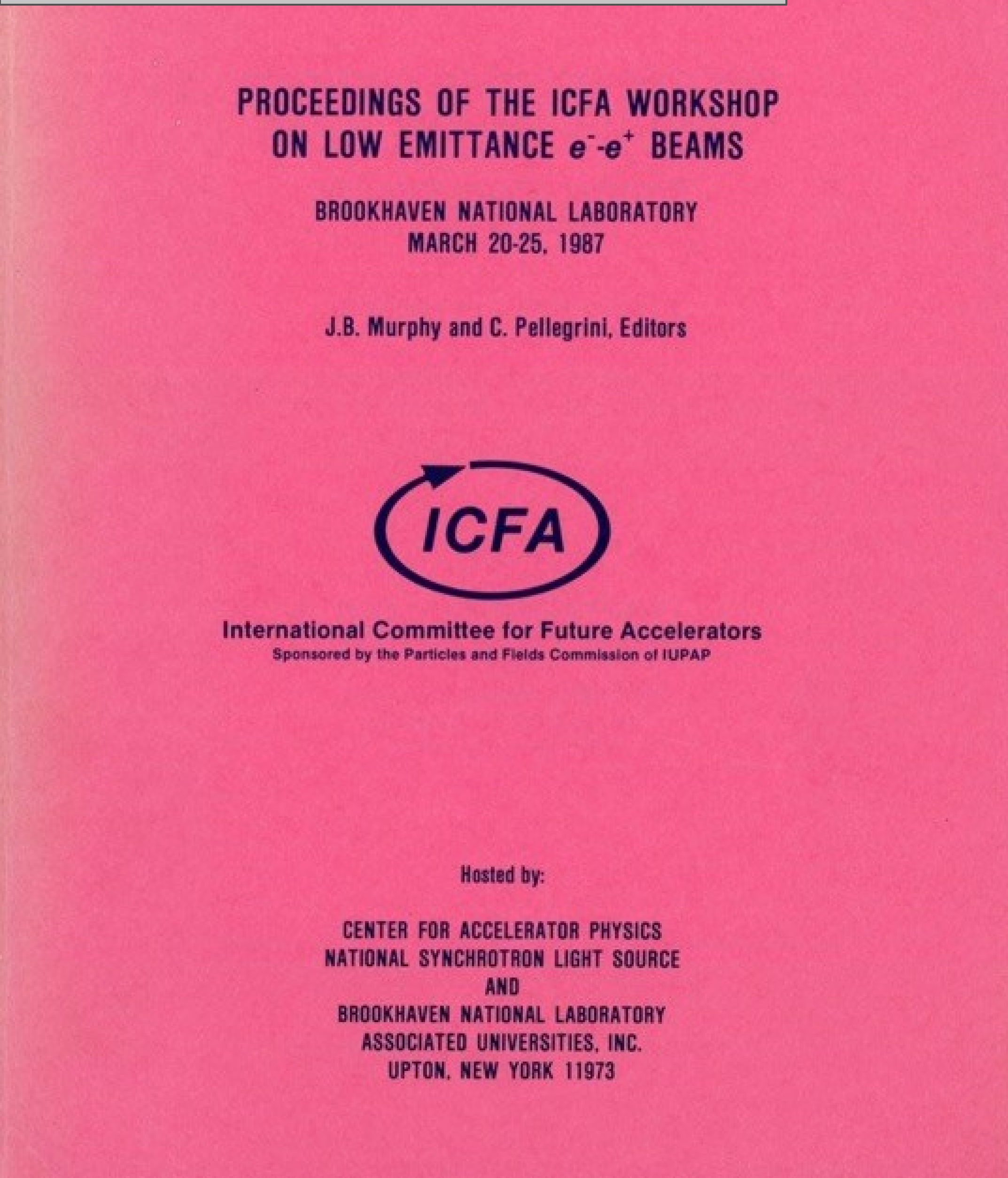


FIG. 1. Schematic of picosecond electron-diffraction apparatus. A streak-camera tube (deflection plates removed) is used to produce the electron pulse. The 25-keV electron pulse passes through the Al specimen and produces a diffraction pattern of the structure with a 20-ps exposure.



X-ray FEL & Ultrafast Electron scattering jointed @ Birth !

High Brightness Electron Injectors
R. Sheffield (LANL)



PROCEEDINGS OF THE ICFA WORKSHOP
ON LOW EMITTANCE e^--e^+ BEAMS

BROOKHAVEN NATIONAL LABORATORY
MARCH 20-25, 1987

J.B. Murphy and C. Pellegrini, Editors

ICFA

International Committee for Future Accelerators
Sponsored by the Particles and Fields Commission of IUPAP

Hosted by:

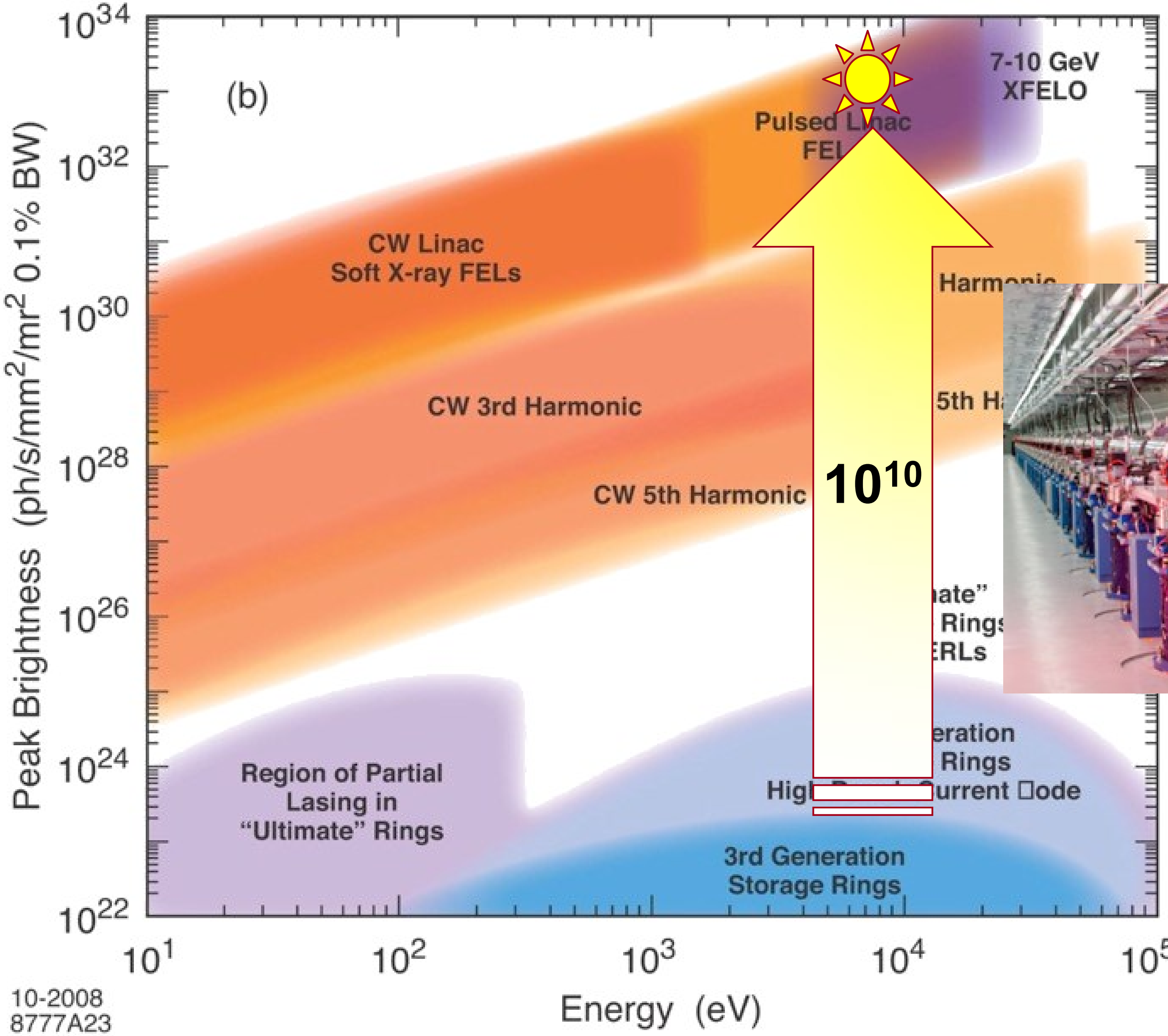
CENTER FOR ACCELERATOR PHYSICS
NATIONAL SYNCHROTRON LIGHT SOURCE
AND
BROOKHAVEN NATIONAL LABORATORY
ASSOCIATED UNIVERSITIES, INC.
UPTON, NEW YORK 11973

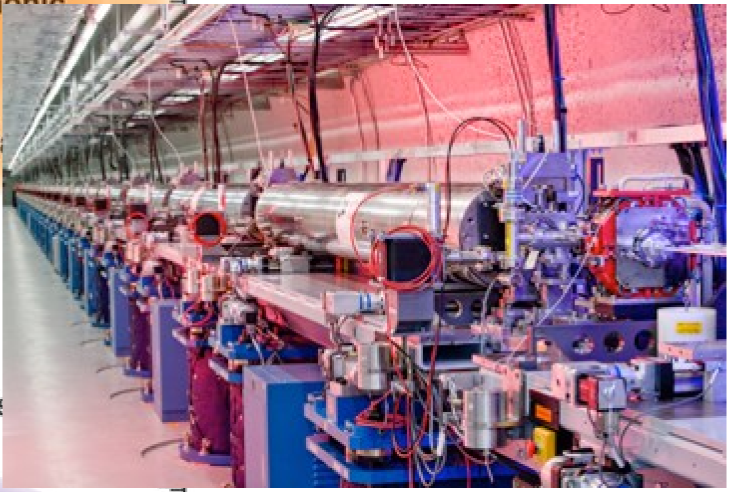
Paradigm Shift: Out go the rings, and in come the Photoinjectors & Linacs as FEL drivers!

BNL/SLAC/UCLA S-Band Gun

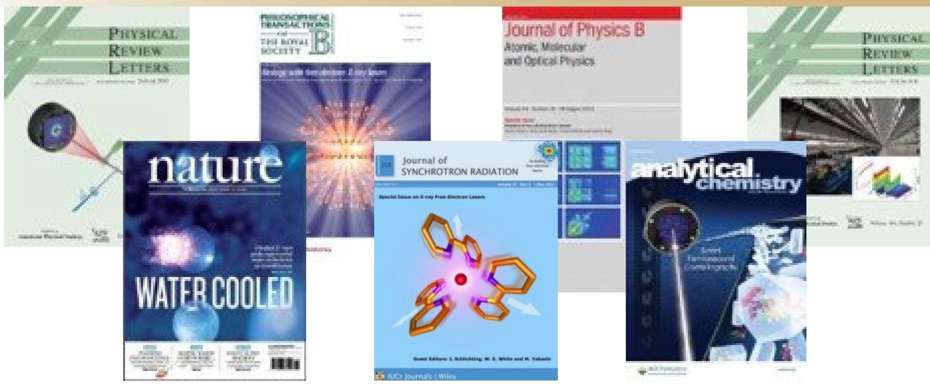
LCLS: A Revolutionary New Source

SLAC

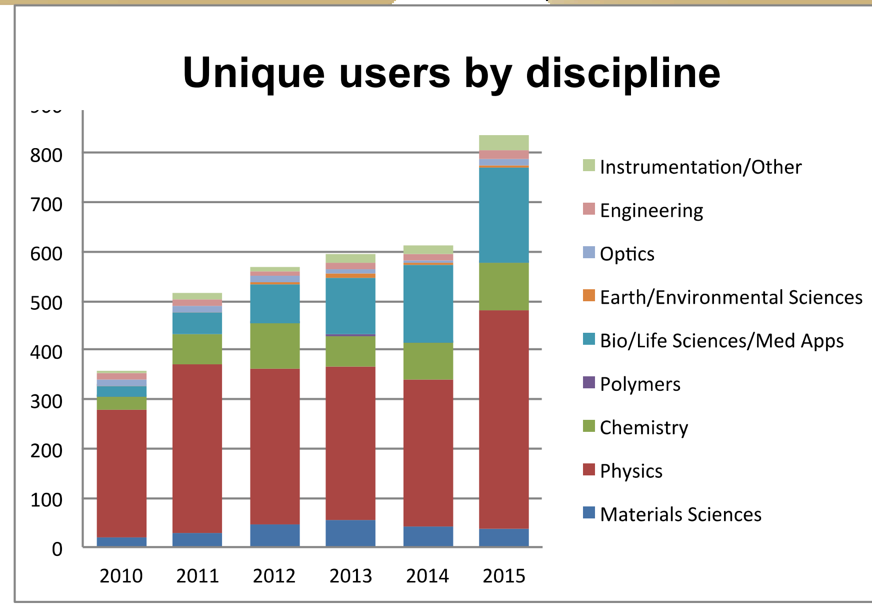


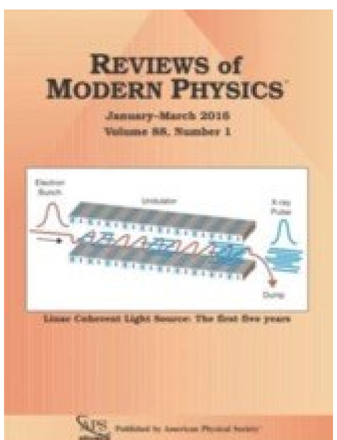


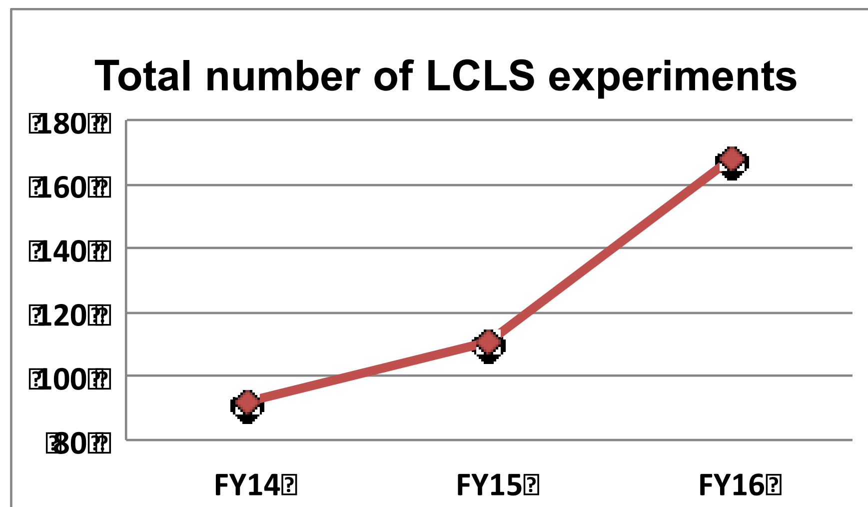
XFEL impact has been substantial



758 papers to date with **168** in high-impact journals, including **32** in ***Science*** or ***Nature*** (~**370** experiments performed to date)

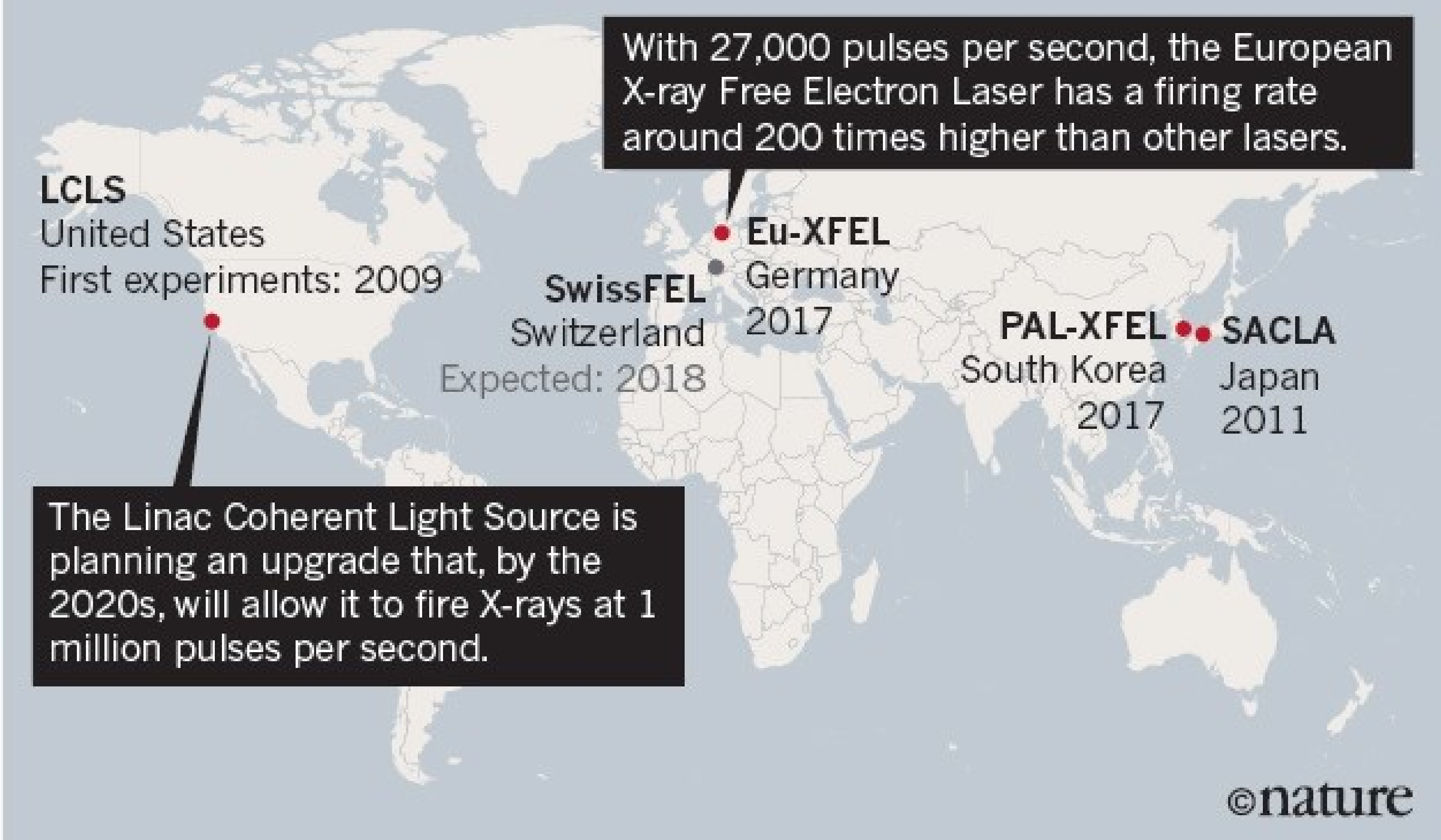






X-RAY LASER GUNS

Four operational facilities worldwide fire bright, X-ray laser light that can determine structures at atomic resolution. Each X-ray flash lasts around 100 femtoseconds — short enough to capture molecular motions.



Applications of Electron Beam Instruments

Electrons microscopes are a $2B annual market. Mostly SEM. From manufacturing to Pharma and essential to R&D
At every National Lab & most universities

E-Beam Wafer Inspection Tools are a $2.4B market

Lithography is a $7B market (mostly optical, but ERL for EUV)

Higher Brightness offers higher throughput, resolution

The Nobel Prize in Chemistry 2017

© Nobel Media. Ill. N. Elmehed

Jacques Dubochet

Prize share: 1/3

© Nobel Media. Ill. N. Elmehed

Joachim Frank

Prize share: 1/3

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Richard Henderson

Prize share: 1/3

The Nobel Prize in Chemistry 2017 was awarded to Jacques Dubochet, Joachim Frank and Richard Henderson *"for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution".*

DOE BES Workshop on Future of Electron Sources

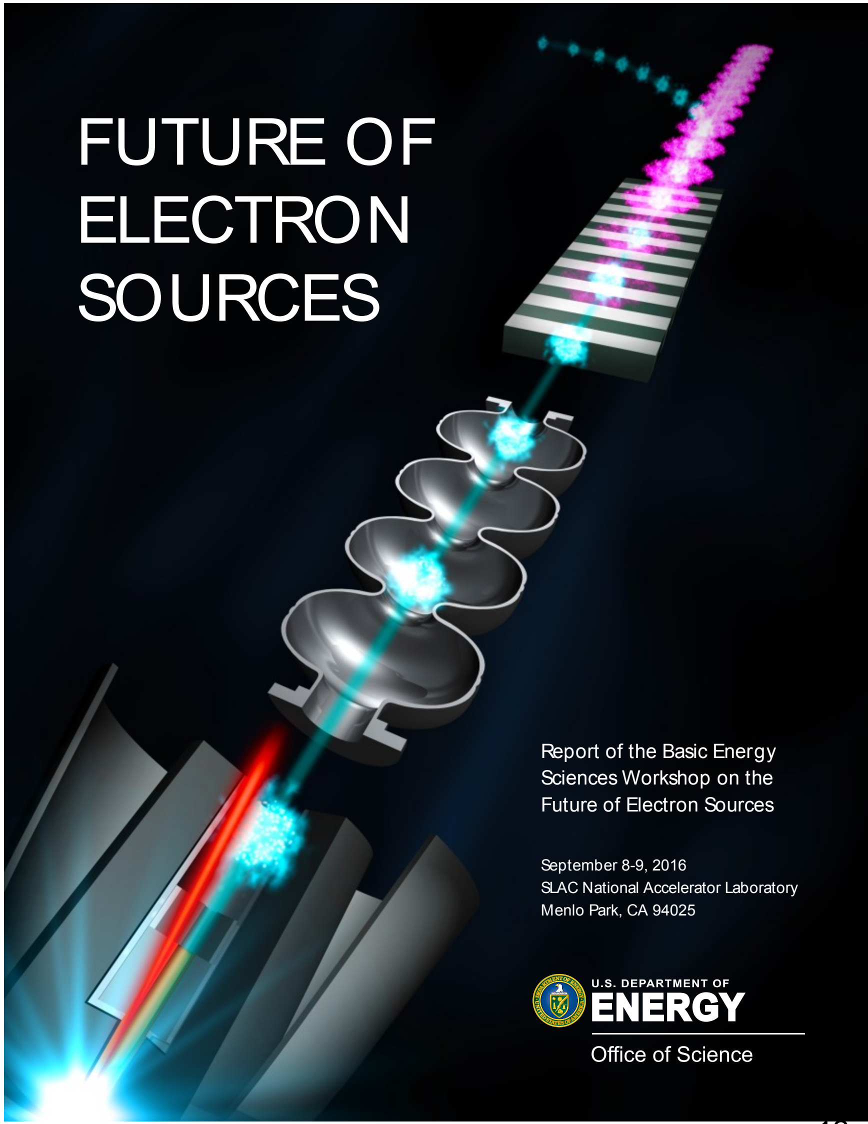
The panel identified the following priority research directions (PRDs):

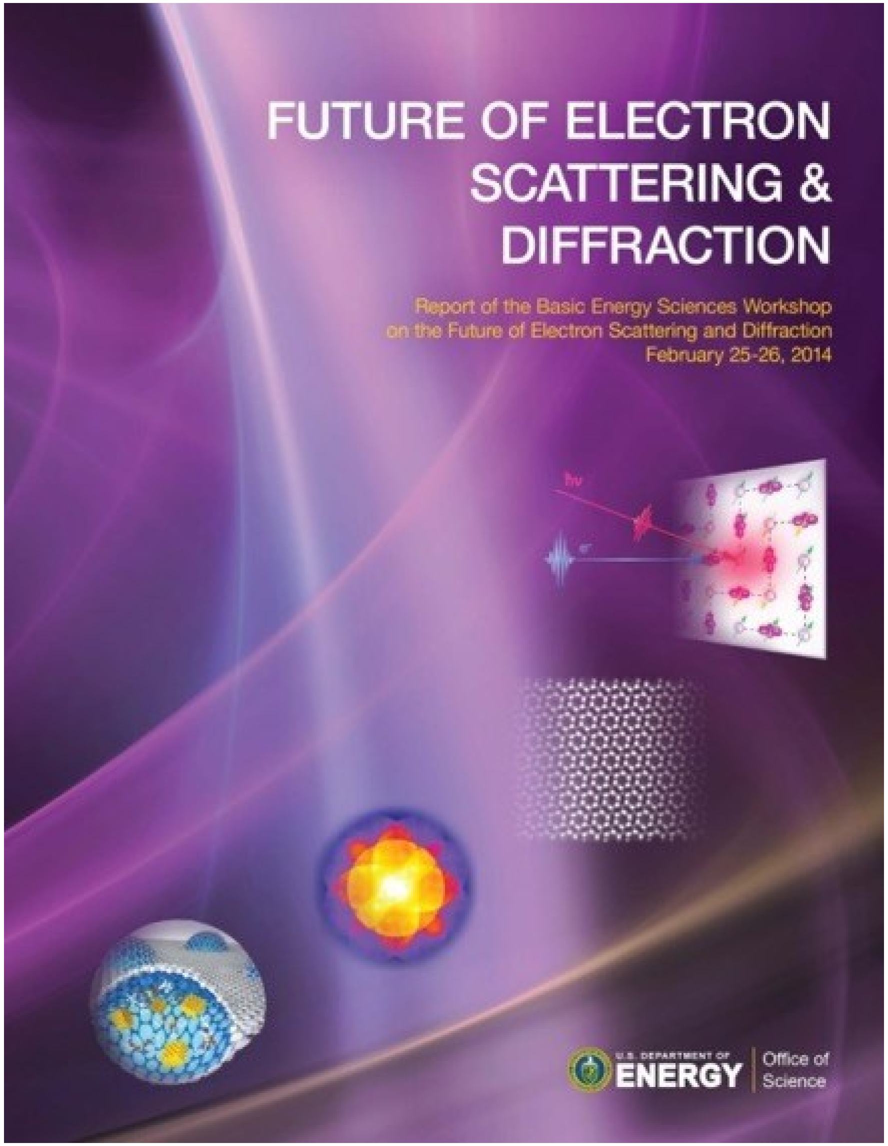
I. **Next generation cathode R&D for high brightness beams.**

II. **CW injector R&D to significantly increase accelerating gradients on the cathode and output beam energy.**

III. **High-gradient R&D for next generation electron sources.**

IV. **R&D in advanced accelerator and beam manipulation concepts.**

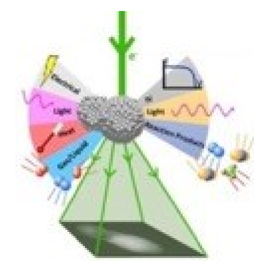


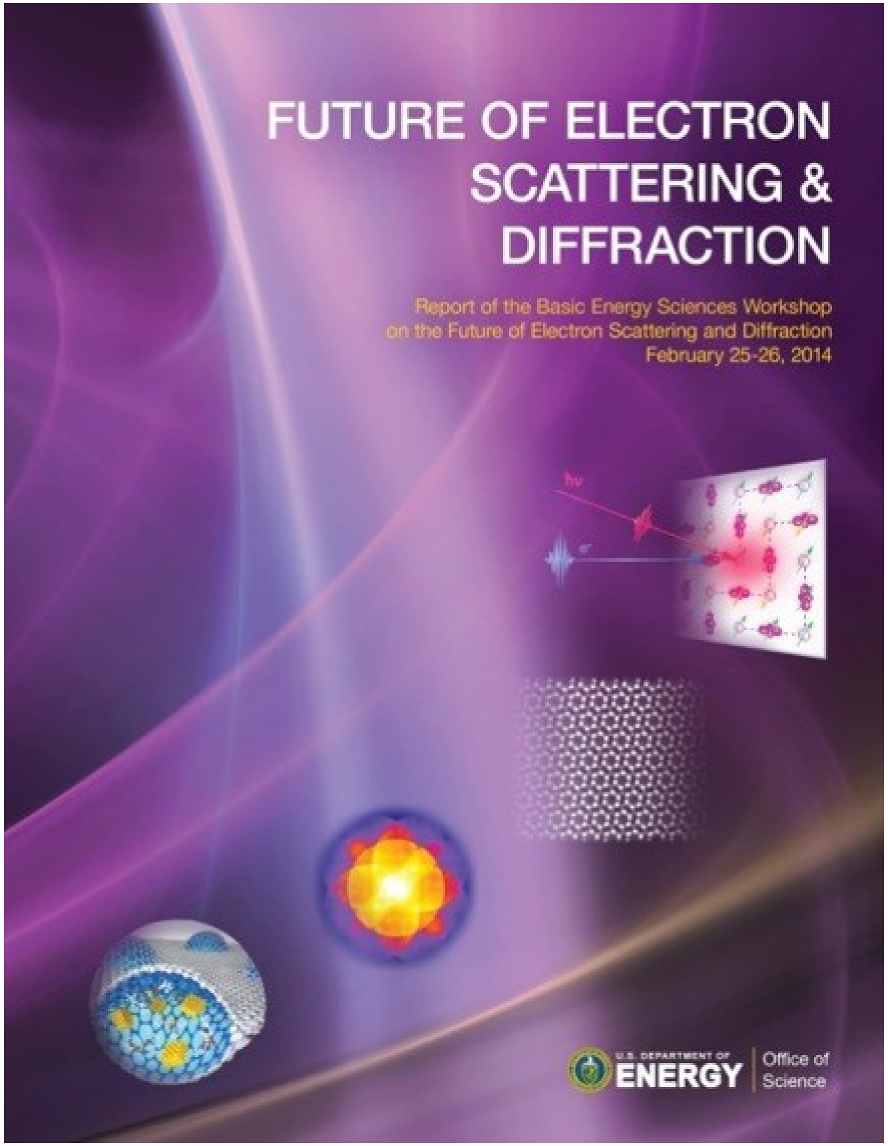


[1] Multidimensional atomic resolution microscope

[2] Ultrafast electron diffraction and microscopy instrument

[3] 'Lab-in-gap' dynamic microscope





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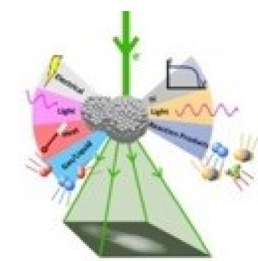
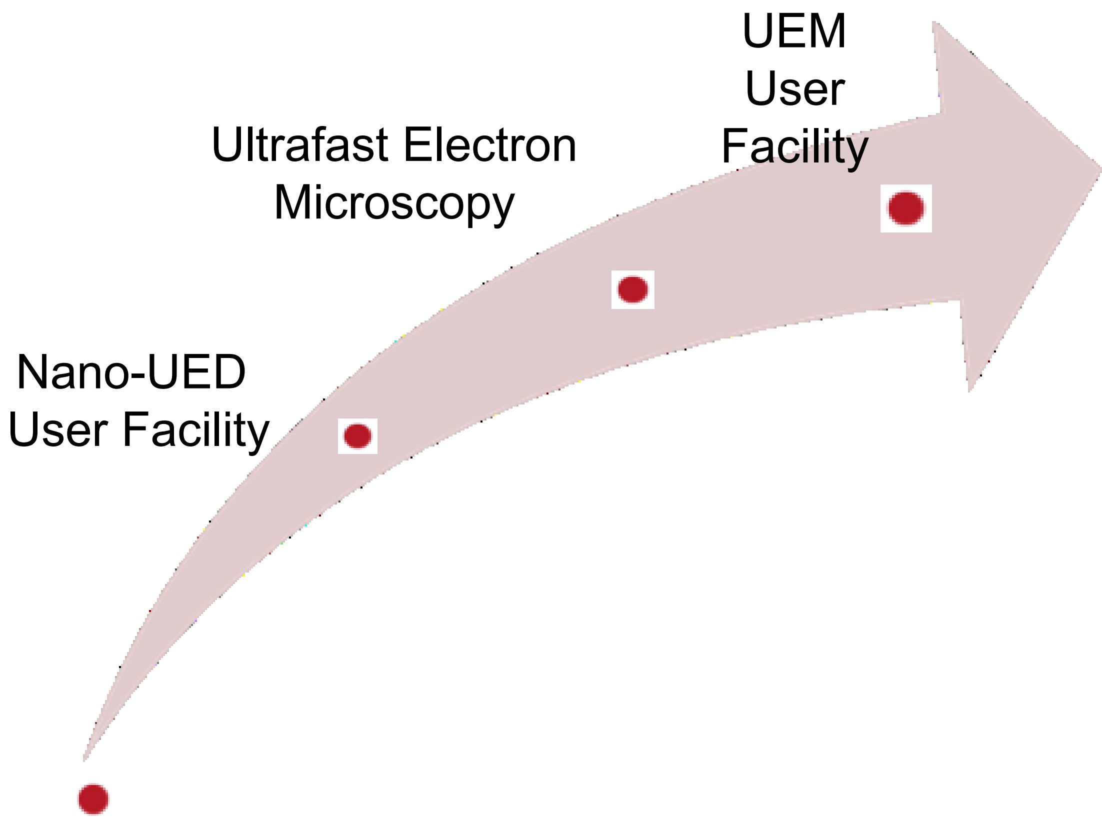
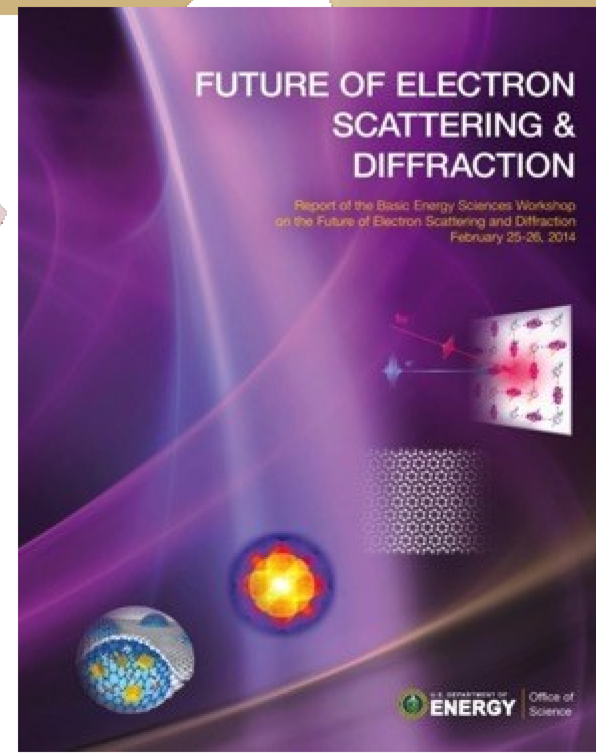


SLAC's Vision for Ultrafast Electron Scattering & Microscopy



The first step: MeV Ultrafast Electron Diffraction (UED)



Recommendation: setup ultrafast electron scattering & microscopy facility

Opportunity to develop the complementarity of x-rays & electrons to access to the "Ultrafast" & "Ultrasmall"

MeV Electron Beams for UED/UEM

PHYSICAL REVIEW E VOLUME 54, NUMBER 4 OCTOBER 1996

Experimental observation of high-brightness microbunching in a photocathode rf electron gun

X. J. Wang, X. Qiu, and I. Ben-Zvi
National Synchrotron Light Source, Brookhaven National Laboratory, Upton, New York 11973
(Received 13 February 1996)

We report the measurement of very short, high-brightness bunches of electrons produced in a photocathode rf gun with no magnetic compression. The electron beam bunch length and the charge distribution along the bunch were measured by passing the energy chirped the electron beam through a momentum selection slit while varying the phase of the rf linac. The bunch compression as a function of rf gun phase and electric field at the cathode were investigated. The shortest measured bunch is 370 ± 100 fs (at 95% of the charge) with 2.5×10^8 electrons (170 A peak current); the normalized rms emittance of this beam was measured to be 0.5π mm mrad and the energy spread is 0.15%. [S1063-651X(96)51110-4]

[1] J. C. Williamson and A. H. Zewail, Proc. Natl. Acad. Sci. USA **88**, 5021 (1991).
[2] J. C. Williamson and G. Mourou, Phys. Rev. Lett. **52**, 2364 (1984).
[3] H. E. Elsayed-Ali and J. W. Herman, Appl. Phys. Lett. **57**, 1508 (1990).
[4] K. J. Kim, S. Chattopadhyay, and C. V. Shank, Nucl. Instrum. Methods Phys. Res. A **341**, 351 (1994).
[5] G. P. Gallerano *et al.*, Nucl. Instrum. Methods Phys. Res. A **358**, 74 (1995).
[6] P. Kung, H. Lihn, and H. Wiedemann, Phys. Rev. Lett. **73**, 967 (1994).
[7] B. E. Carlsten and S. J. Russell, Phys. Rev. E **53**, R2072 (1996).

MeV Ultrafast Electrons for UED &UEM

PHYSICAL REVIEW E VOLUME 54, NUMBER 4 OCTOBER 1996

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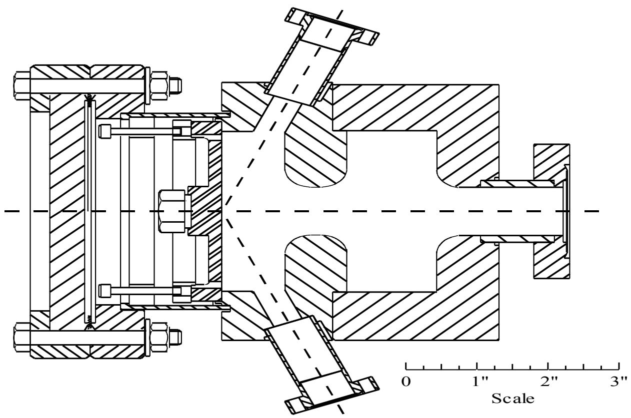
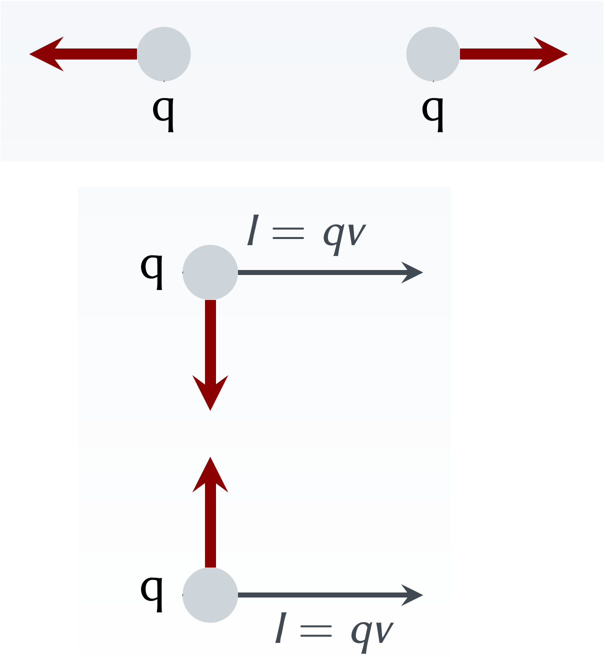
- ✓ **Better temporal resolution? (Jitter is concern)**
- ❖ Beam quality good enough?
- ❖ Signal too week & Sample damage?
- ❖ **More Expensive? True**

Photocathode RF gun and Space charge effects

- **High acceleration field.**
- **Laser control temporal and space distributions.**
- **Cathode technology.**



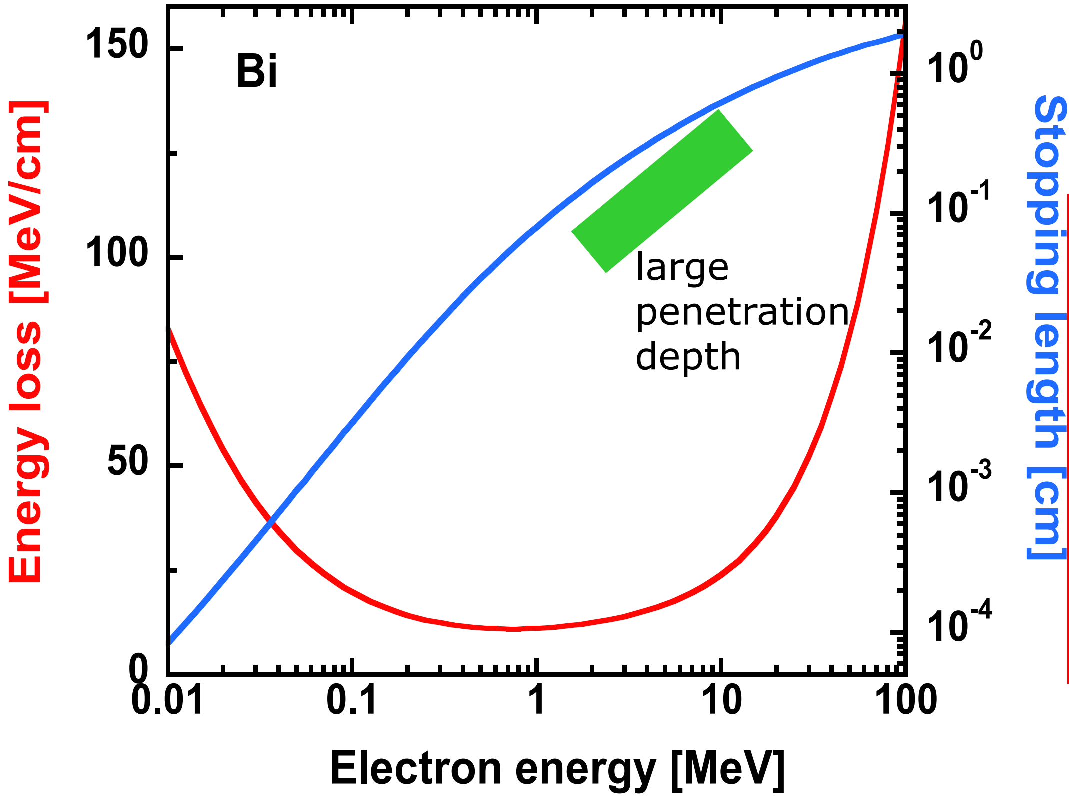
Photocathode RF Gun



Space charge effect: **$(1/(\beta^2\gamma^3)$**

Why diffraction with MeV electrons?

Space charge effect: $(1/(\beta^2\gamma^3)$



"thick" samples

kinematic diffraction
@ 3.2 MeV, MFP ~ 20 nm
@ 55 KeV, MFP ~ 3 nm

"really" flat Ewald-sphere

physics.nist.gov/PhysRefData/Star/Text/ESTAR.html

Timeline

Apr 2014 MeV UED launched

June 2014 bunker cleared

August 2014 UED beamline installed

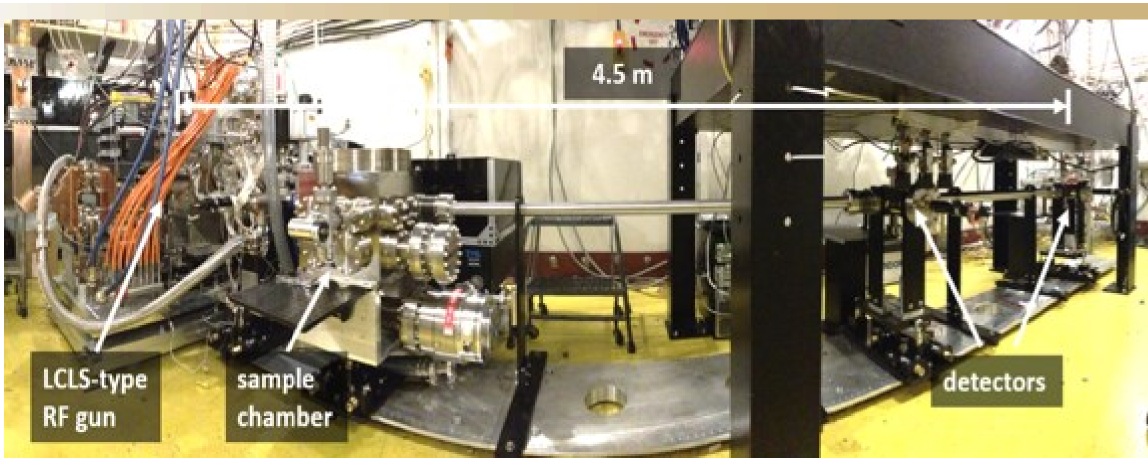
Aug 22 2014 first beam

March 2015 gas phase UED

March 2016 single-shot MeV UED

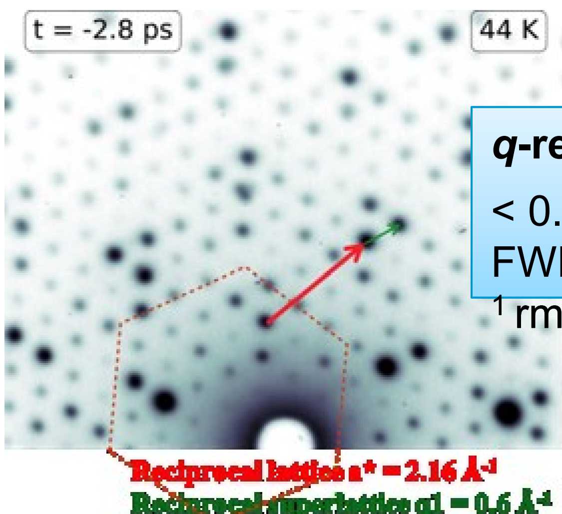
June 2017 THz

SLAC MeV UED Summary



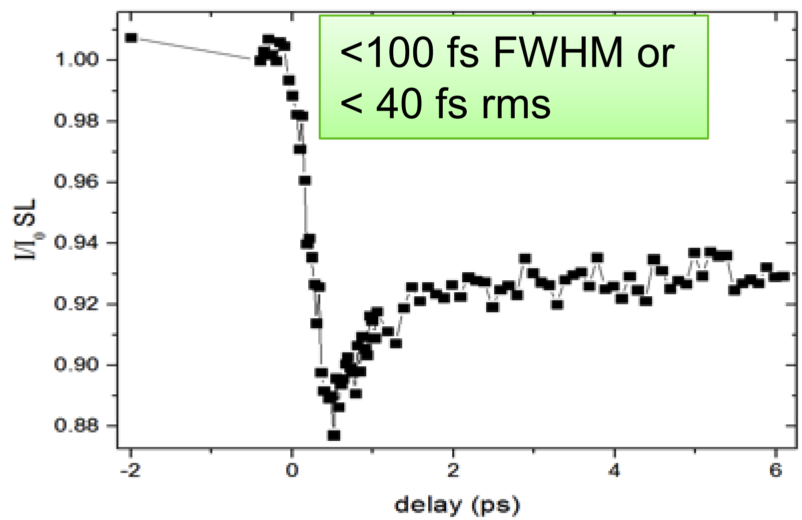
Typical beam parameters

Parameters	Values
rep. rate	SS - 180 Hz
beam energy	2 - 4 MeV
e^- /bunch	10^4-10^6
emittance	2 - 20 nm
bunch length	<40 fs (rms)



***q*-resolution**

< 0.17 $Å^{-1}$ FWHM or 0.07 $Å^{-1}$ rms

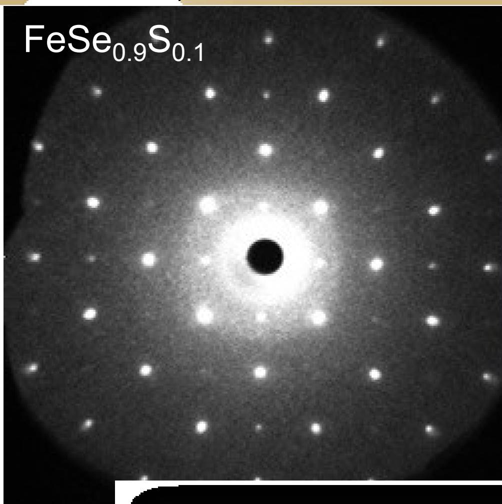


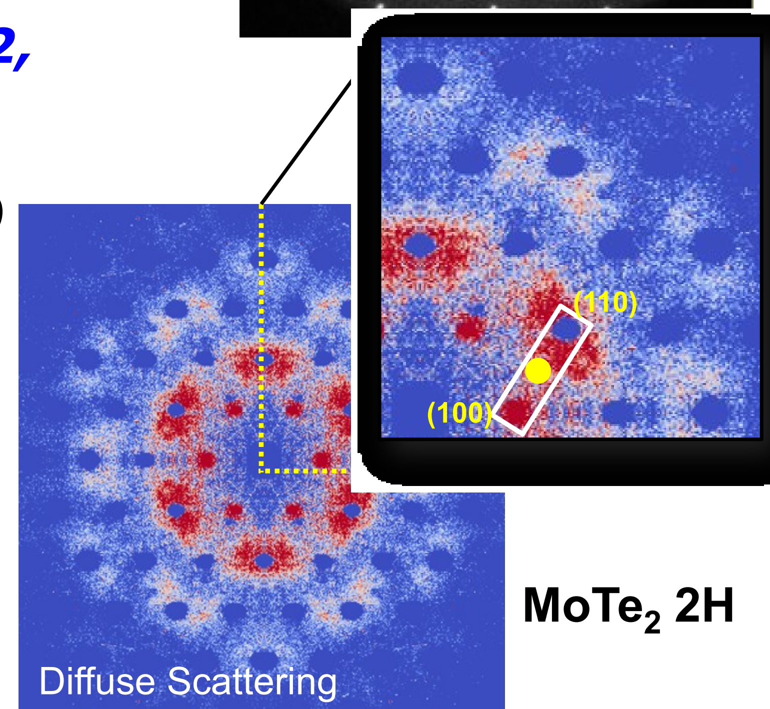
<100 fs FWHM or < 40 fs rms

https://portal.slac.stanford.edu/sites/ard_public/tfd/ued/Pages/default.aspx

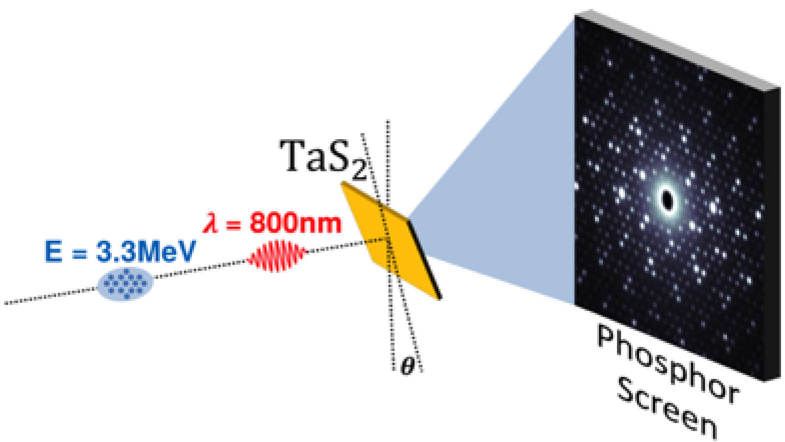
Ultrafast science: *material science*

- ***Nano-scale materials (Bi, FePt, nano-porous Au, Cr-Cu heterostrucutre)***
- ***2-D Materials(MoS_2 $MoSe_2$ WTe_2)***
- ***Diffuse scattering (Au, Ni)***
- ***Quantum Materials (Bi2212, 1T-TaS_2, LSMO, $SrTiO_3$, $TiSe_2$)***
- ***Functional material(Perovskite, PbI2, Vo_2)***
- ***Warm dense matter (W, Au, Copper)***



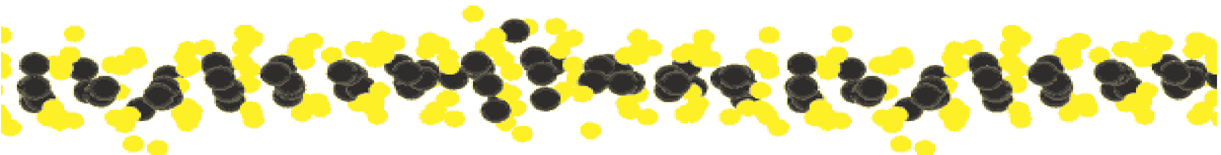


MoTe$_2$ 2H

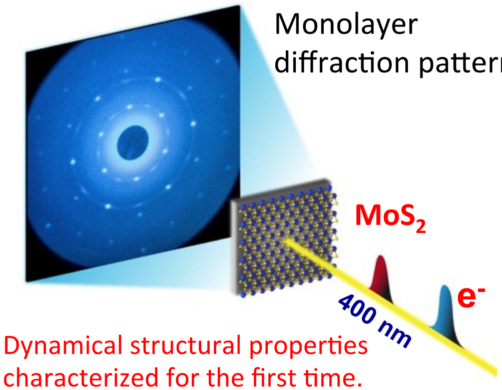


Ultrafast material science enabled by MeV-UED

✓ *2-D Materials*

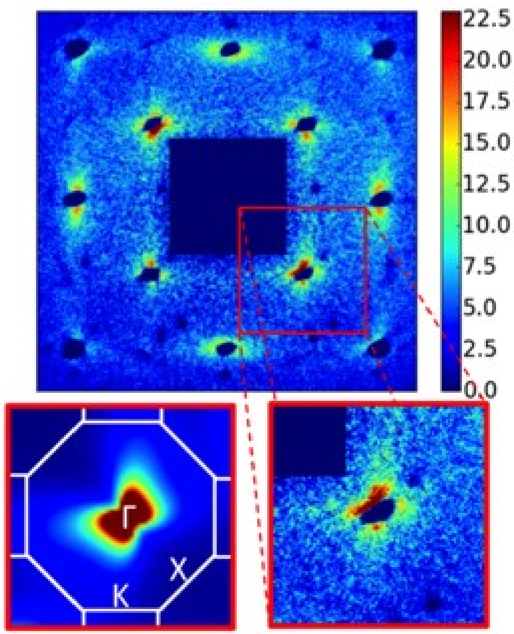


E. M. Mannebach *et al.*, *Nano Letters*, 31 August 2015



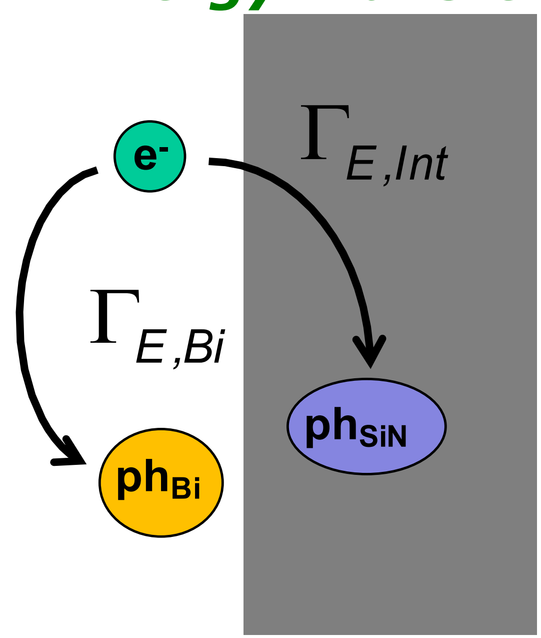
Dynamical structural properties characterized for the first time.

✓ *Diffuse scattering*



T. Chase et al, *APL* **108,** 041909 (2016).
[DOI: 10.1063/1.4940981]

✓ *Energy Transfer*

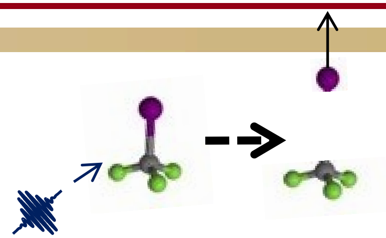


New J. Phys. 17, 113047 (2015).
Struct. Dyn. 4, 054501 (2017)

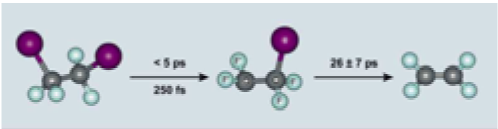
Photo-chemistry

Photodissociation:

CF_3I; $C_2F_4I_2$



CF_3I dissociation



$C_2F_4I_2$ dissociation

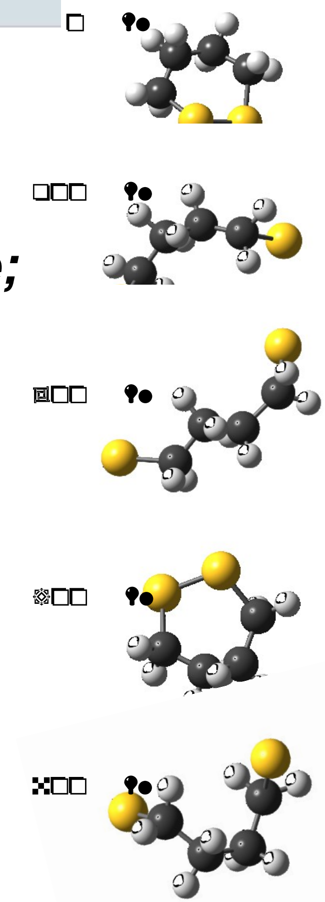
Roam-type reaction:

Nitrobenzene

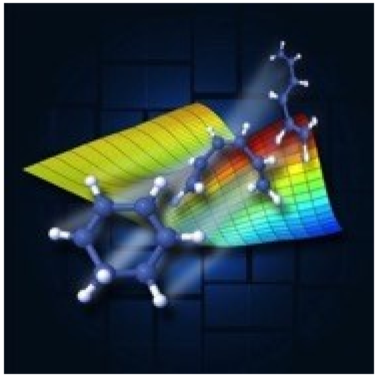
Ring-opening reaction:

1,2 – Dithiane; cis-Stilbene Oxide;

1,3 - Cyclohexadiene



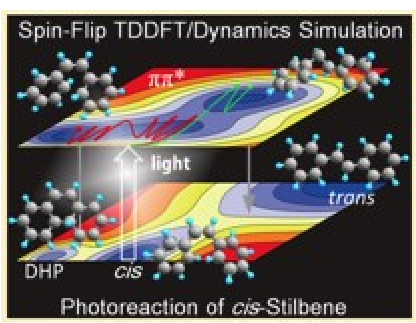
Dithiane



1,3 – Cyclohexadiene (CHD) ring-opening

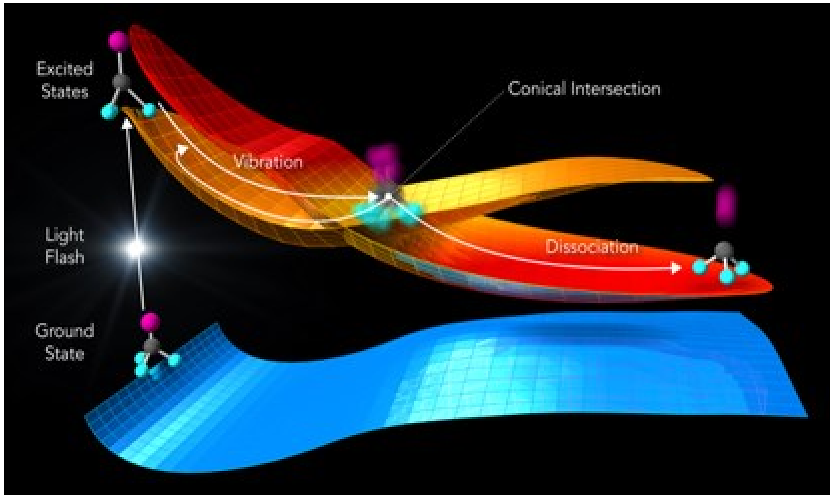
Photoisomerization:

cis-Stilbene



Stilbene Isomerization

Science enabled by the high-brightness electron beams



Bond-breaking & nuclear wavepacket passing through conical intersections (*Science 361 64–67 (2018)*)

CHEMICAL PHYSICS

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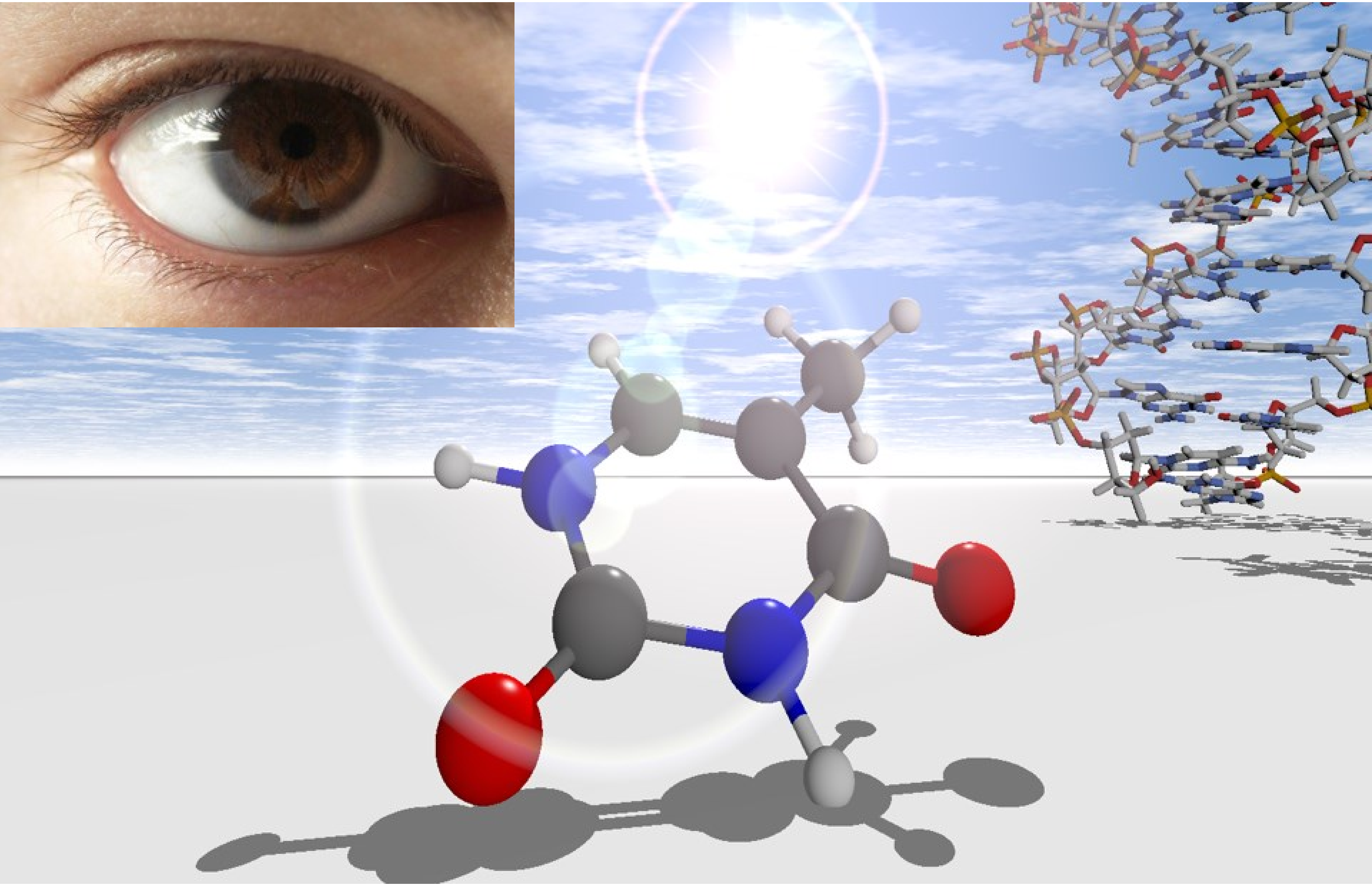
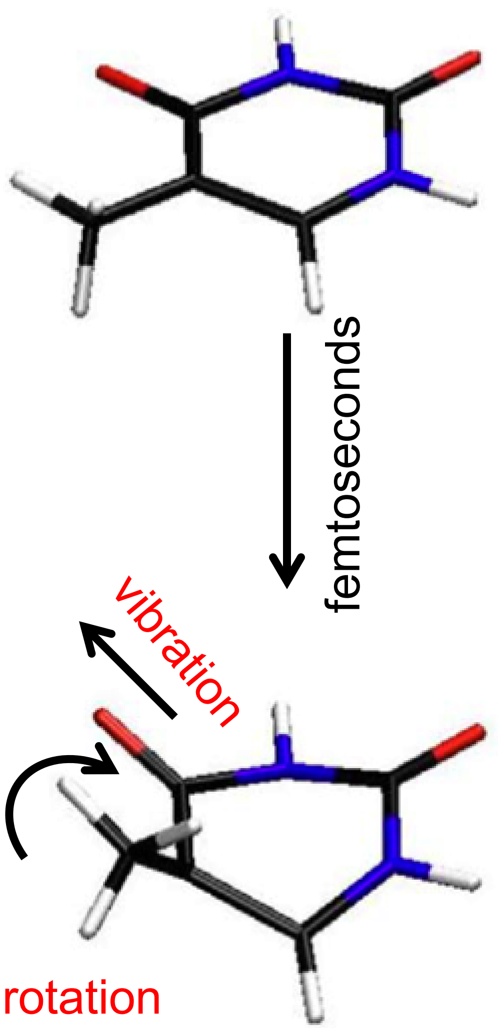
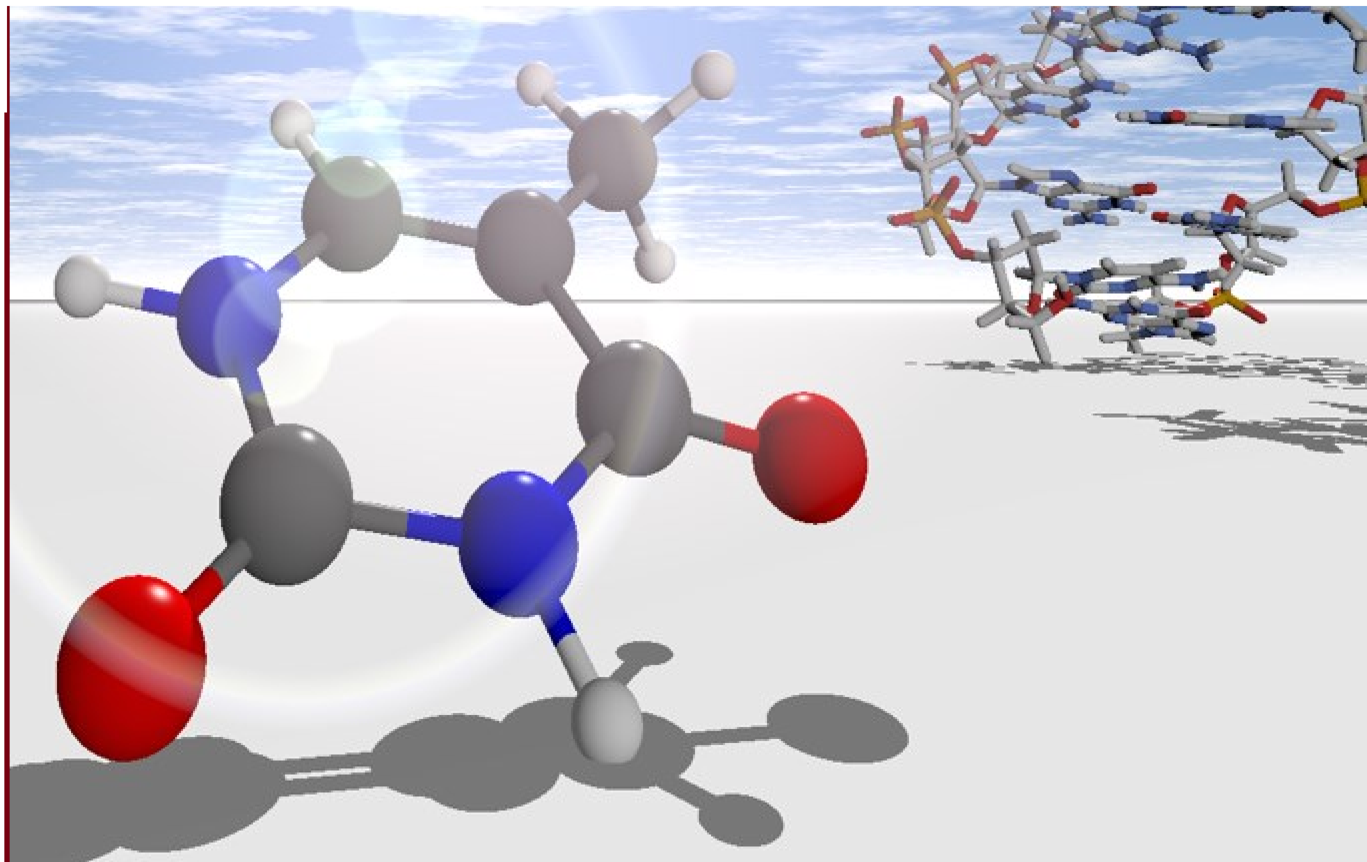
Photoenergy conversion in molecules



Photoenergy conversion in molecules

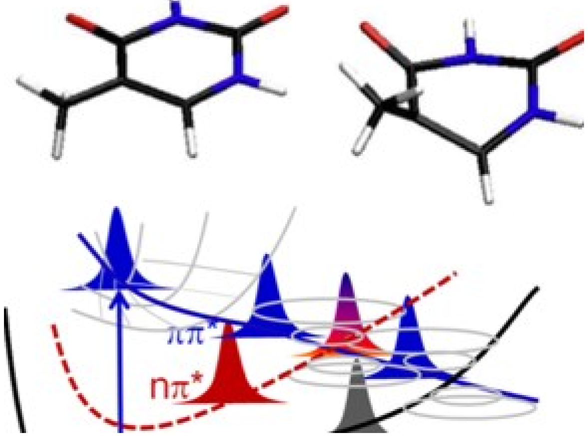


- molecules transfer photon energy selectively into bond change, charge transfer or heat
- correlated motion of electrons and nuclei necessary
- example: nucleobases transfer UV photonenergy into heat
- this is possible due to certrain motions of the nuclei - highly controersial what that looks like

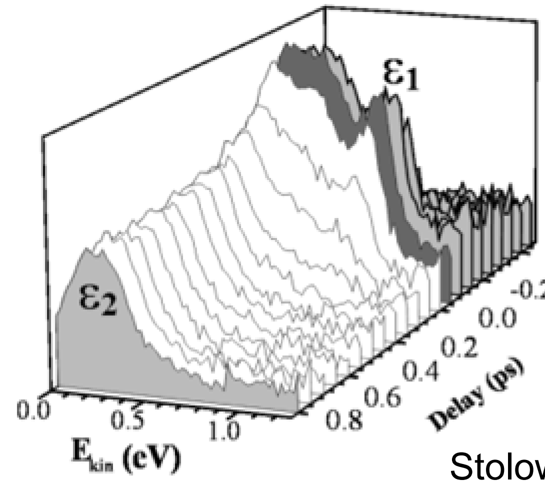


Photochemistry - gas phase diffraction

Comparison to high level ab initio
Rule out interaction with environment

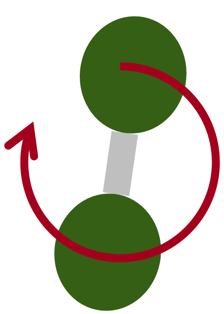


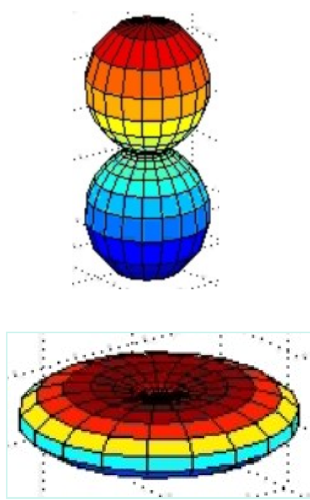
Comparison to photoelectron spectra



Stolow, Bragg, Neumark, Chem. Rev. 2004

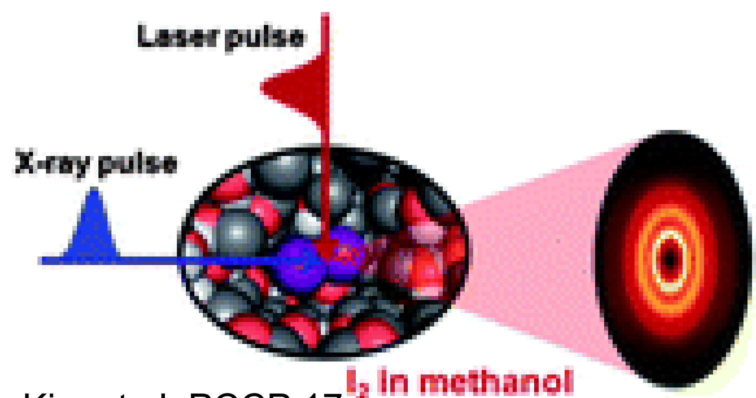
Field free alignment / quantum manipulation





Courtesy of Markus Gühr

No background from solvent



Kim et al, PCCP 17, 8633 (2015)

ARTICLE

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Diffractive imaging of a rotational wavepacket in nitrogen molecules with femtosecond megaelectronvolt electron pulses

Jie Yang[1], Markus Guehr[2,3], Theodore Vecchione[4], Matthew S. Robinson[1], Renkai Li[4], Nick Hartmann[4], Xiaozhe Shen[4], Ryan Coffee[4], Jeff Corbett[4], Alan Fry[4], Kelly Gaffney[4], Tais Gorkhover[4], Carsten Hast[4], Keith Jobe[4], Igor Makasyuk[4], Alexander Reid[4], Joseph Robinson[4], Sharon Vetter[4], Fenglin Wang[4], Stephen Weathersby[4], Charles Yoneda[4], Martin Centurion[1] & Xijie Wang[4]

Selected for a Viewpoint in *Physics*

PRL 117, 153002 (2016) PHYSICAL REVIEW LETTERS week ending 7 OCTOBER 2016

Diffractive Imaging of Coherent Nuclear Motion in Isolated Molecules

Jie Yang,[1] Markus Guehr,[2,3,*] Xiaozhe Shen,[4] Renkai Li,[4] Theodore Vecchione,[4] Ryan Coffee,[4] Jeff Corbett,[4] Alan Fry,[4] Nick Hartmann,[4] Carsten Hast,[4] Kareem Hegazy,[4] Keith Jobe,[4] Igor Makasyuk,[4] Joseph Robinson,[4] Matthew S. Robinson,[1] Sharon Vetter,[4] Stephen Weathersby,[4] Charles Yoneda,[4] Xijie Wang,[4,†] and Martin Centurion[1,‡]

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(Received 19 March 2016; published 3 October 2016)

CHEMICAL PHYSICS

Imaging CF_3I conical intersection and photodissociation dynamics with ultrafast electron diffraction

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Conical intersections play a critical role in excited-state dynamics of polyatomic molecules because they govern the reaction pathways of many nonadiabatic processes. However, ultrafast probes have lacked sufficient spatial resolution to image wave-packet trajectories through these intersections directly. Here, we present the simultaneous experimental characterization of one-photon and two-photon excitation channels in isolated CF_3I molecules using ultrafast gas-phase electron diffraction. In the two-photon channel, we have mapped out the real-space trajectories of a coherent nuclear wave packet, which bifurcates onto two potential energy surfaces when passing through a conical intersection. In the one-photon channel, we have resolved excitation of both the umbrella and the breathing vibrational modes in the CF_3 fragment in multiple nuclear dimensions. These findings benchmark and validate ab initio nonadiabatic dynamics calculations.

Light-induced molecular dynamics usually cannot be described within the framework of the Born-Oppenheimer approximation. The picture of nuclear motion on a single adiabatic potential energy surface (PES), determined by treating the fast-moving electrons separately from the slower nuclei, breaks down wherever two or more adiabatic PESs come close in energy (1, 2). At the crossing point of PESs, the degeneracy is lifted along at least two internal degrees of freedom, and the resultant conical intersection guides efficient radiationless transitions between electronic states at specific nuclear configurations (3). Examples of important nonadiabatic reactions include photosynthesis (4), retinal isomerization in vision (5), ultraviolet-induced DNA damage (6), and formation of vitamin D (7).

Several experimental methods have been developed for studying nonadiabatic dynamics through conical intersections (8–13). Among these, time-averaged photofragment imaging can identify distinct spectral features of nonadiabatic coupling (8, 9) but does not allow the observation of dynamics in real time. Time-resolved laser spectroscopy is the most widely used real-time method for following electronic dynamics, but nuclear dynamics can only be inferred on the basis of an indirect comparison with simulated transient spectroscopic features (11–14). In addition, comparison with theoretical predictions requires explicit modeling of the probing process, which can be more complex than the nonadiabatic dynamics in question. Recent developments in both x-ray (15, 16) and electron-based (17, 18) time-resolved diffraction techniques open an opportunity for direct imaging of conformational changes during chemical reactions—molecular movies with atomic resolution in space and time. Despite the great importance of nonadiabatic dynamics through conical intersections, spatiotemporal resolution has not been sufficient to image a coherent nuclear wave packet traversing a conical intersection with time-resolved diffraction techniques.

The nonadiabatic transitions of molecules between different PESs are inherently quantum mechanical. A wide variety of computational methods can be used to simulate dynamics through conical intersections. For small systems, nonadiabatic dynamics can be treated with exact full quantum dynamics (19) and the highly accurate multiconfigurational time-dependent Hartree approximation (20). For larger systems, semiclassically motivated approaches such as Tully's surface hopping (21), Meyer-Miller formalism (22), or ab initio multiple spawning (AIMS) (23) are routinely used. Although simulations can provide rich details of the dynamics through conical intersections, nontrivial approximations at many different stages of the calculations are required, even for relatively small systems. Therefore, confirmation with experimental measurements is crucial.

Here, we report the direct imaging of both conical intersection dynamics and photodissociation dynamics of gas-phase CF_3I molecules with atomic resolution by use of ultrafast gas-phase electron diffraction (UGED). A 264.5-nm pump laser pulse initiates two photoexcitation channels: a one-photon transition to the dissociative A band and a two-photon transition to the $[5p\pi^3, {}^2\Pi_{3/2}](7s)$ (24) Rydberg state (referred to as 7s below) (25), as illustrated in Fig. 1. The adiabatic dissociation dynamics through A-band excitation of CF_3I and its analog, CH_3I, have been studied extensively (26–29). We created a multidimensional movie of the structural changes in the CF_3 fragment immediately after iodide dissociation, with a precision of ±0.01 Å in bond length and ±1° in bond angle. Various groups have studied the two-photon transition into the 7s channel by using pump-probe photoelectron and photo-ion spectroscopy (25, 30–32). These studies identified the decay time scale and anisotropy of fragment ions, but the reaction pathway remained elusive. Specifically, it was only a speculation that a nearby ion-pair state might be involved in the reaction dynamics (31). We have mapped out the nuclear wave-packet trajectory in real space, which directly shows wave-packet bifurcation though a conical intersection. Through cross-verification with AIMS simulations, we have clarified that the $\sigma\sigma^*$ state correlates asymptotically to a CF_3^+–I^- ion-pair state (referred to as IP) at large C–I separation, and that this state plays a key role in this channel. The reaction pathway is predominantly determined by the nonadiabatic coupling between IP and multiple states: the 7s and $[5p\pi^3, {}^2\Pi_{1/2}](6s)$ Rydberg states (referred to as 6s below) and valence states.

The UGED experimental setup is shown in Fig. 2A, which is described in detail in (33, 34) and the supplementary materials. For diffraction pattern analysis, we used a two-dimensional (2D) Fourier transform followed by Abel inversion to convert data from momentum space to real space. This procedure returns a pair-distribution-function (PDF) that reports all the interatomic distances, as explained in Fig. 2, B to E.

The one-photon channel preferentially excites molecules with the C–I axis aligned along the laser polarization. This results in a $\cos^2\theta$ angular distribution of excited-state molecules, where θ is the angle between the C–I bond and the laser polarization (Fig. 2, B and C). In this case, C–I and F–I pairs mostly appear in the parallel direction ($PDF_{\parallel}$), and the C–F and F–F pairs preferentially appear in the perpendicular direction ($PDF_{\perp}$). The two-photon channel corresponds to a perpendicular excitation ($\sin^4\theta$ distribution) (Fig. 2, D and E). In this case, C–I and F–I pairs preferentially appear in $PDF_{\perp}$, whereas C–F and F–F slightly favor $PDF_{\parallel}$. This analysis simultaneously

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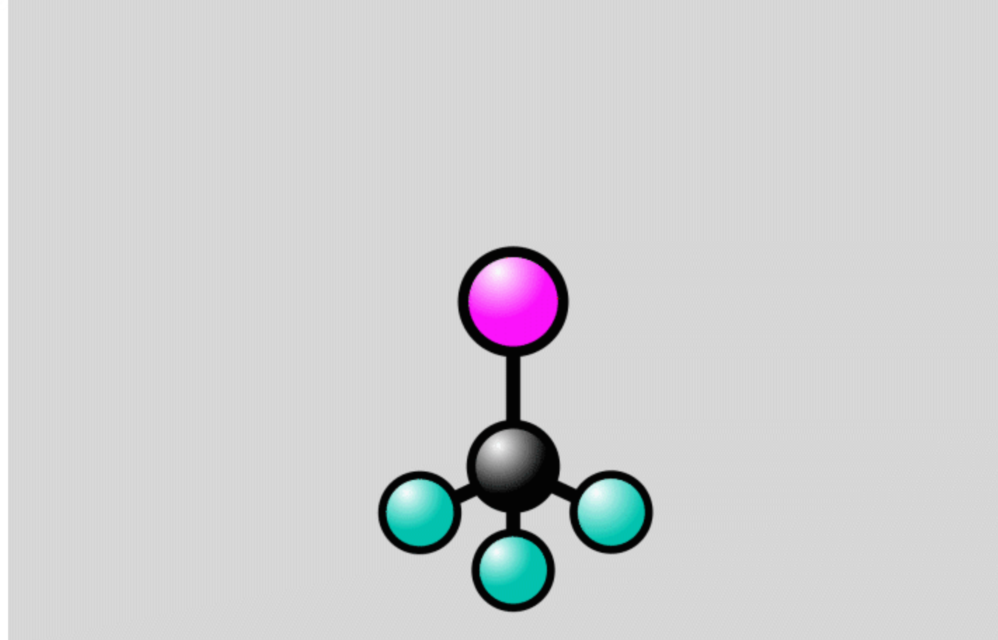
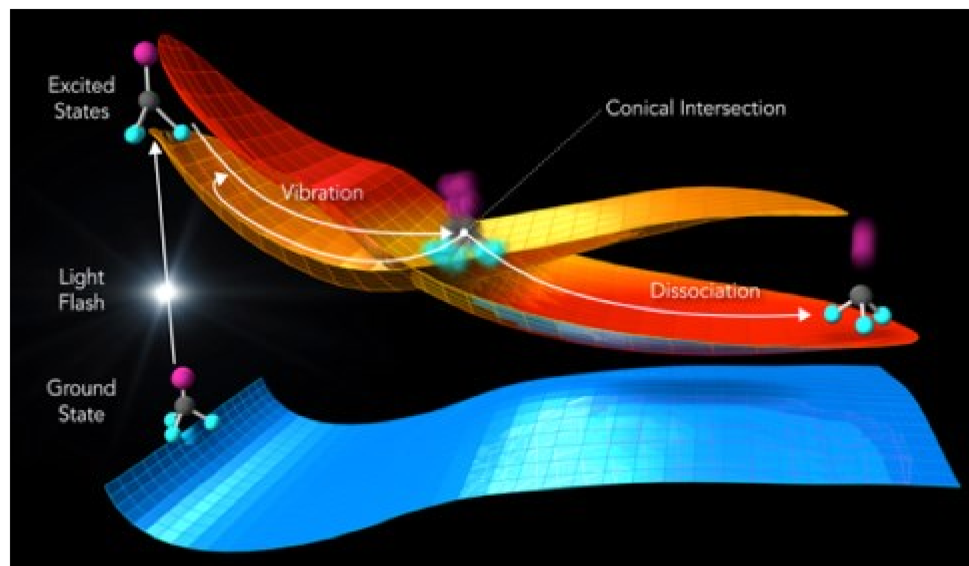
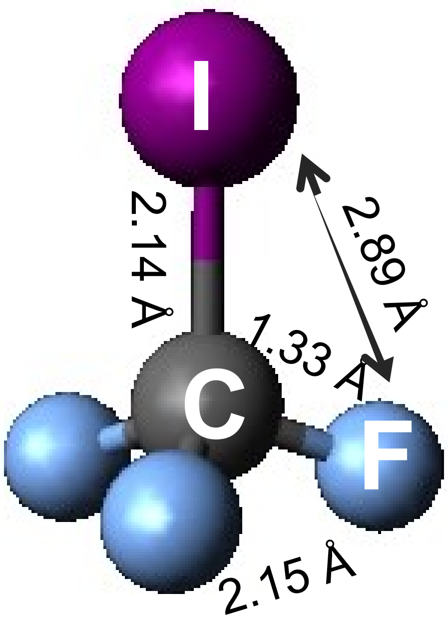
*Corresponding author. Email: jieyang@slac.stanford.edu (J.Y.); toddmartinez@stanford.edu (T.J.M.); martin.centurion@unl.edu (M.C.); wangxj@slac.stanford.edu (X.W.)



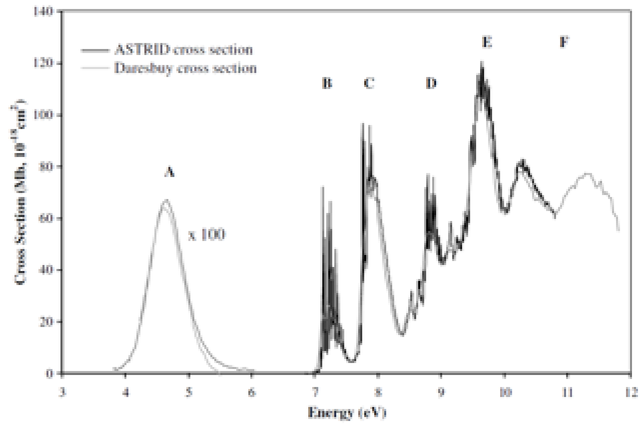


Introduction to CF_3I

CF_3I Structure

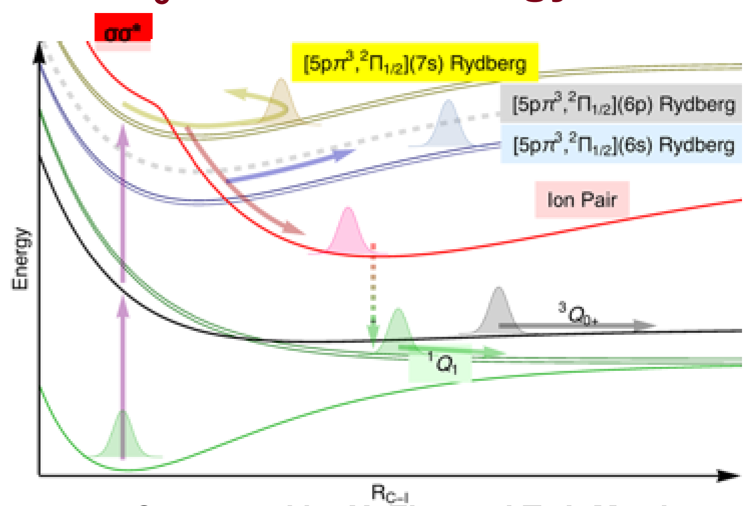


CF_3I Absorption Spectrum



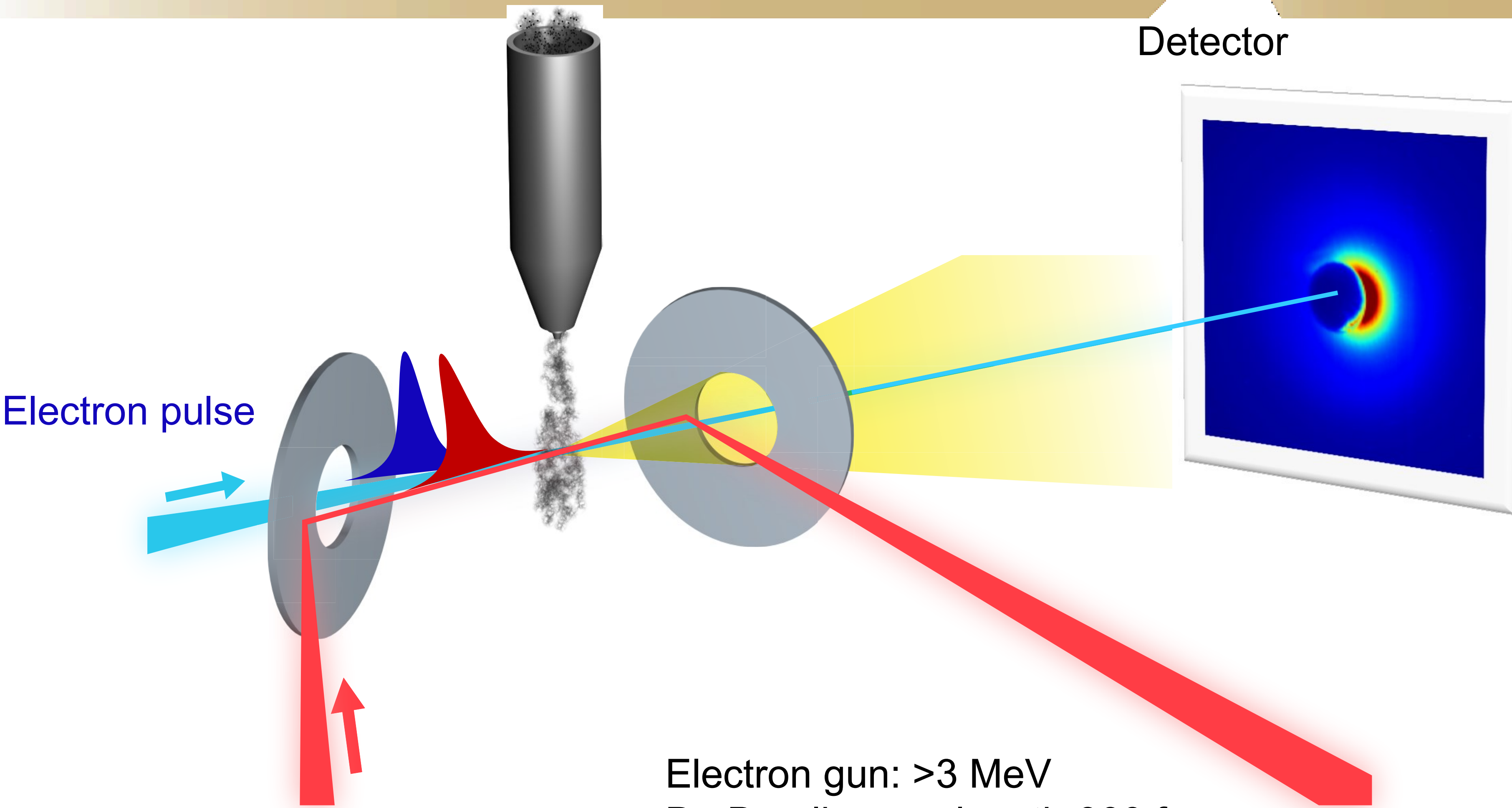
S. Eden et al. Chem. Phys. 323 (2006) 313–333

CF_3I Potential Energy Surface



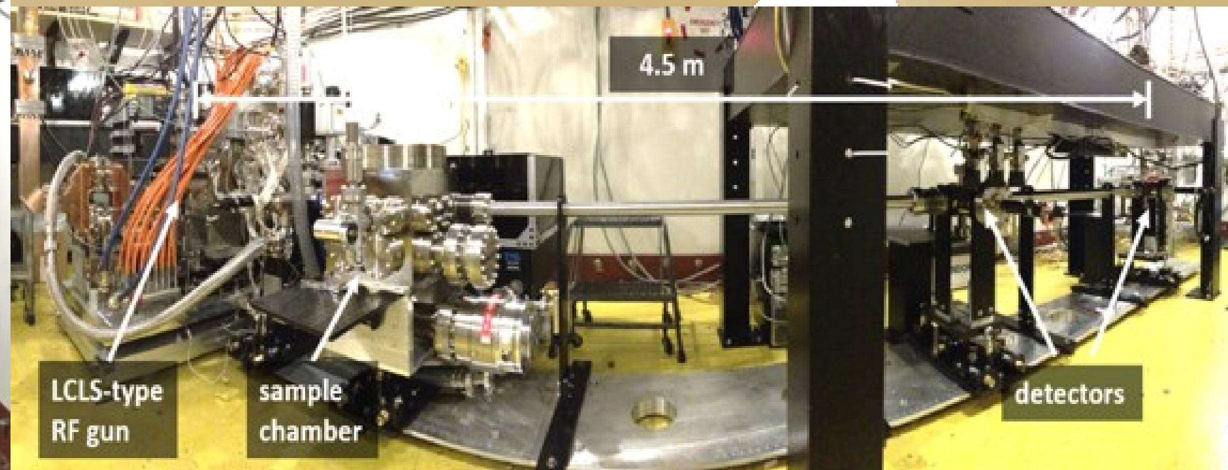
Calculated by X. Zhu and T. J. Martinez

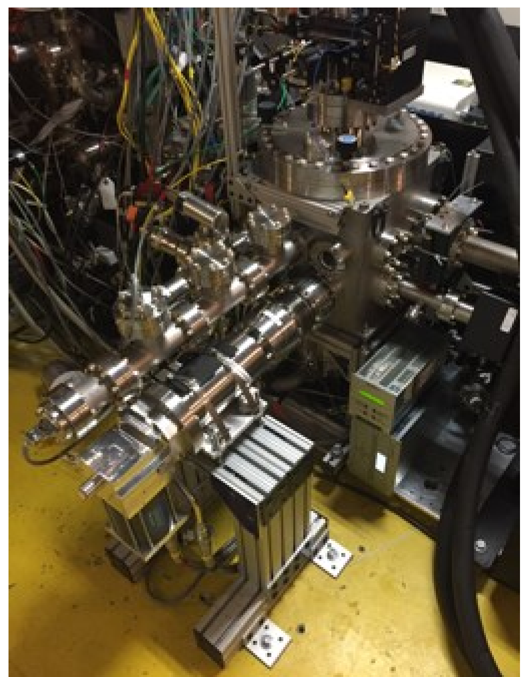
Experimental setup

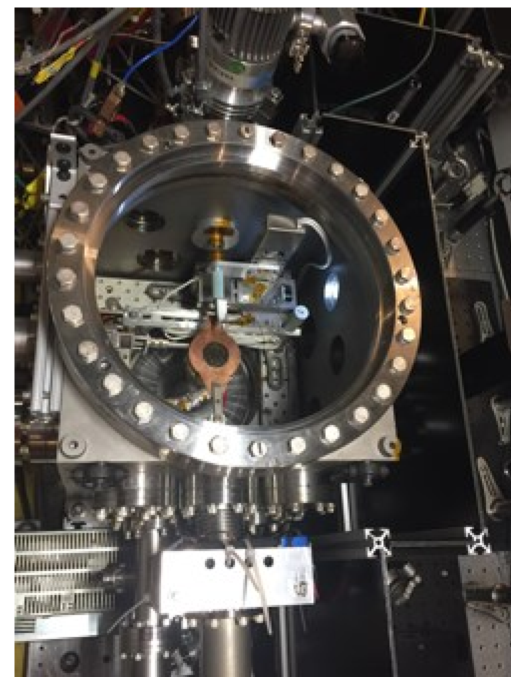


Electron gun: >3 MeV
De Broglie wavelength 300 fm
β=0.97, Negligible group velocity mismatch
10^5 Electrons per pulse

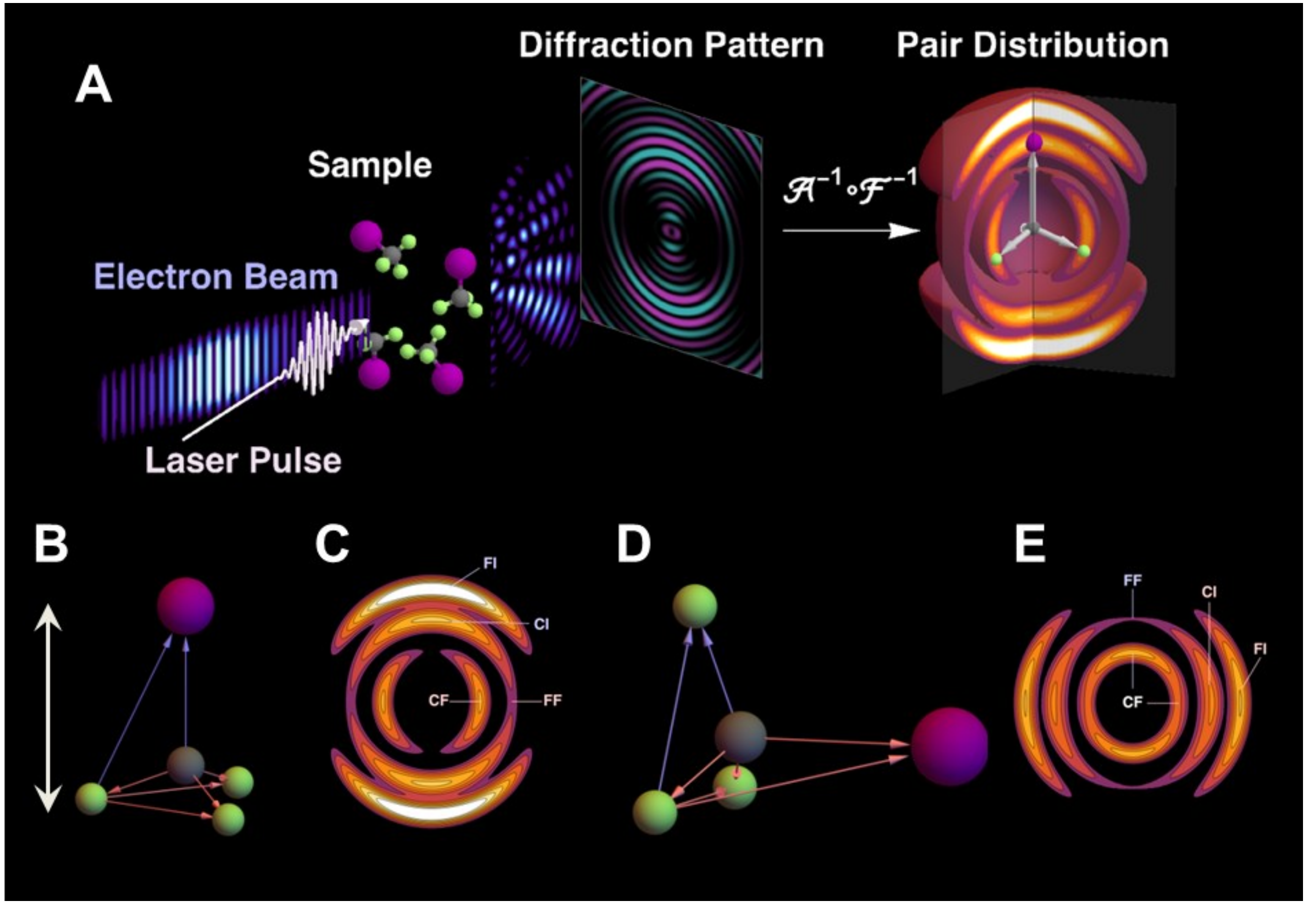
Experimental setup



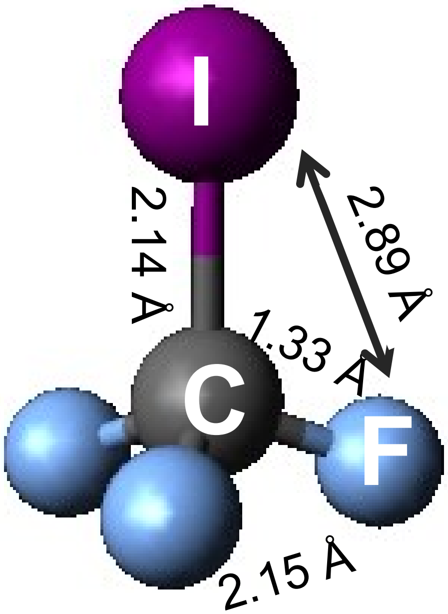




Anisotropy comes from Photoselection rule

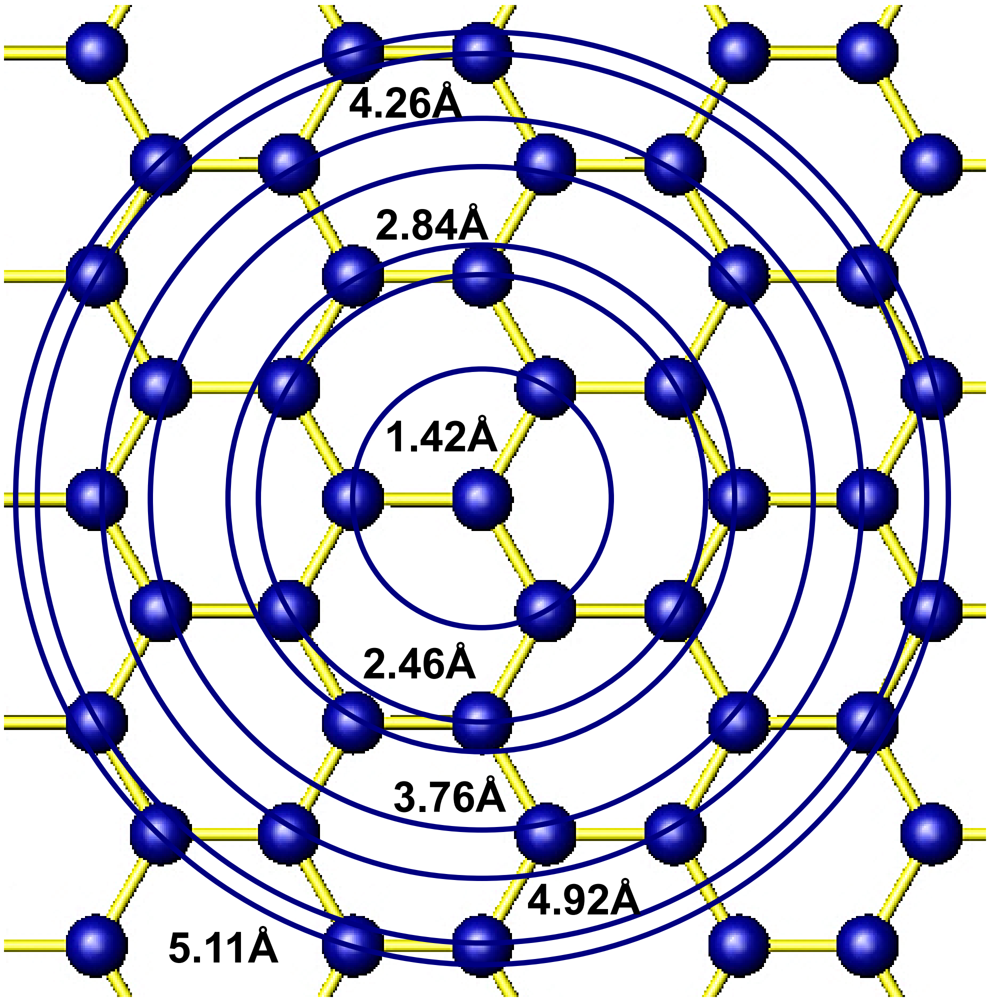


CF_3I Structure

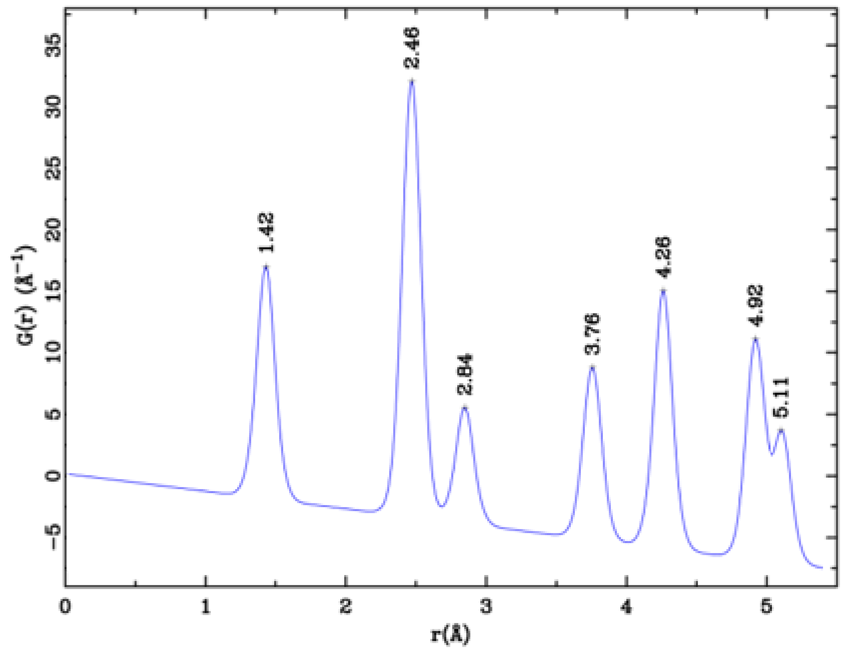


J. Yang et al, Science 361 64–67 (2018).

What is a Pair Distribution Function (PDF)?

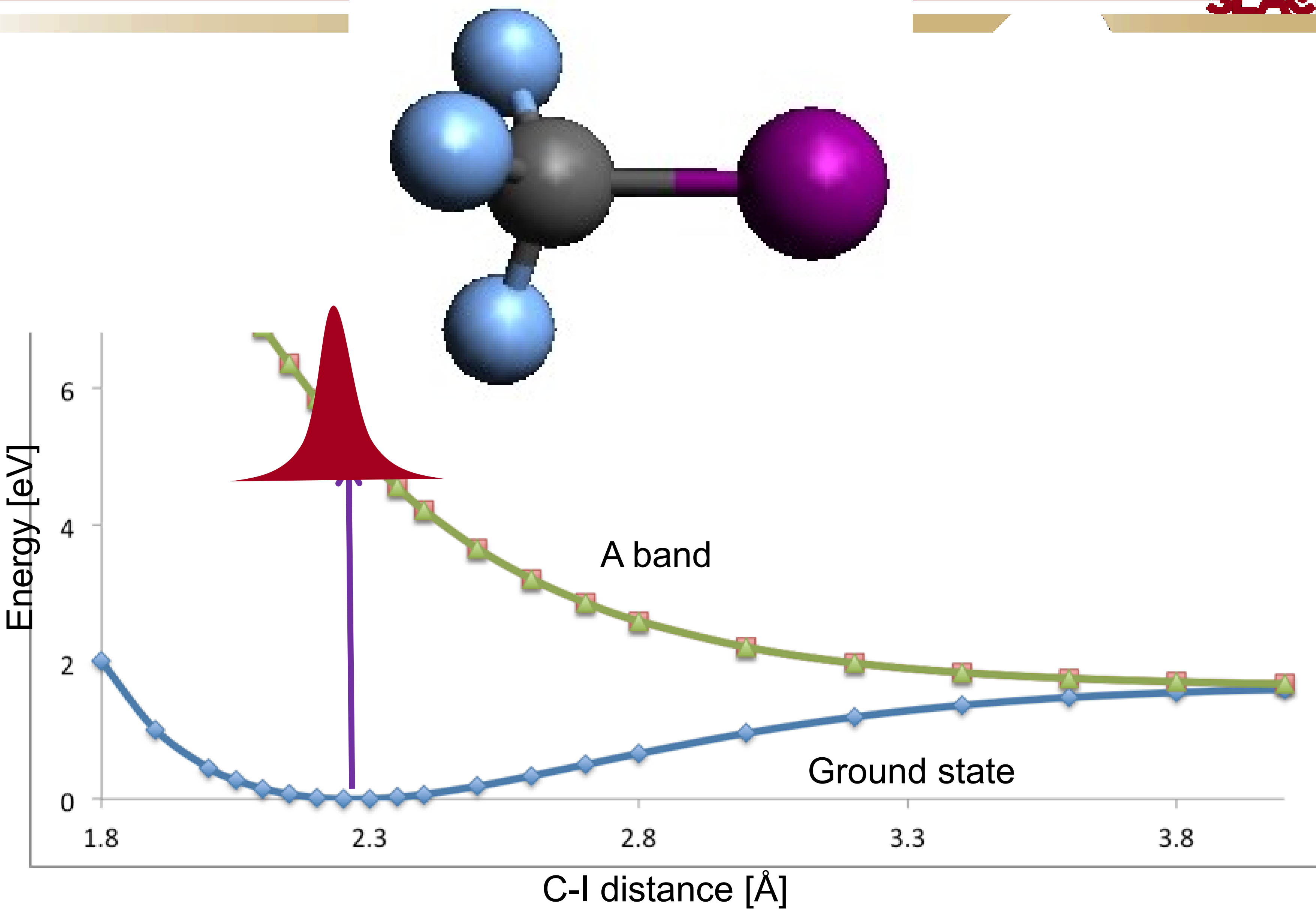


Pair distribution function (PDF) gives the probability of finding an atom at a distance "r" from a given atom.

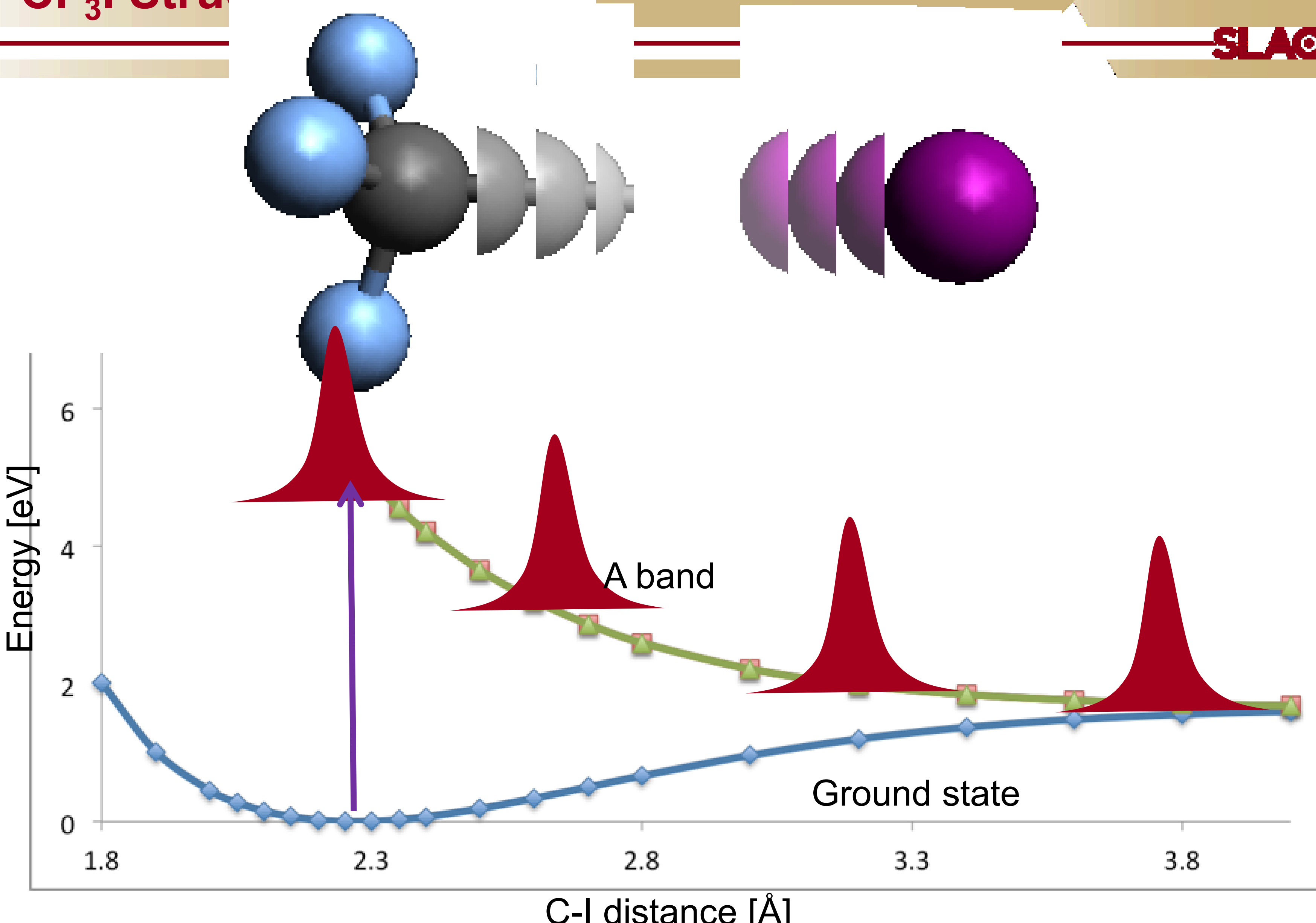


Thomas Proffen of ORNL, NXS 2015

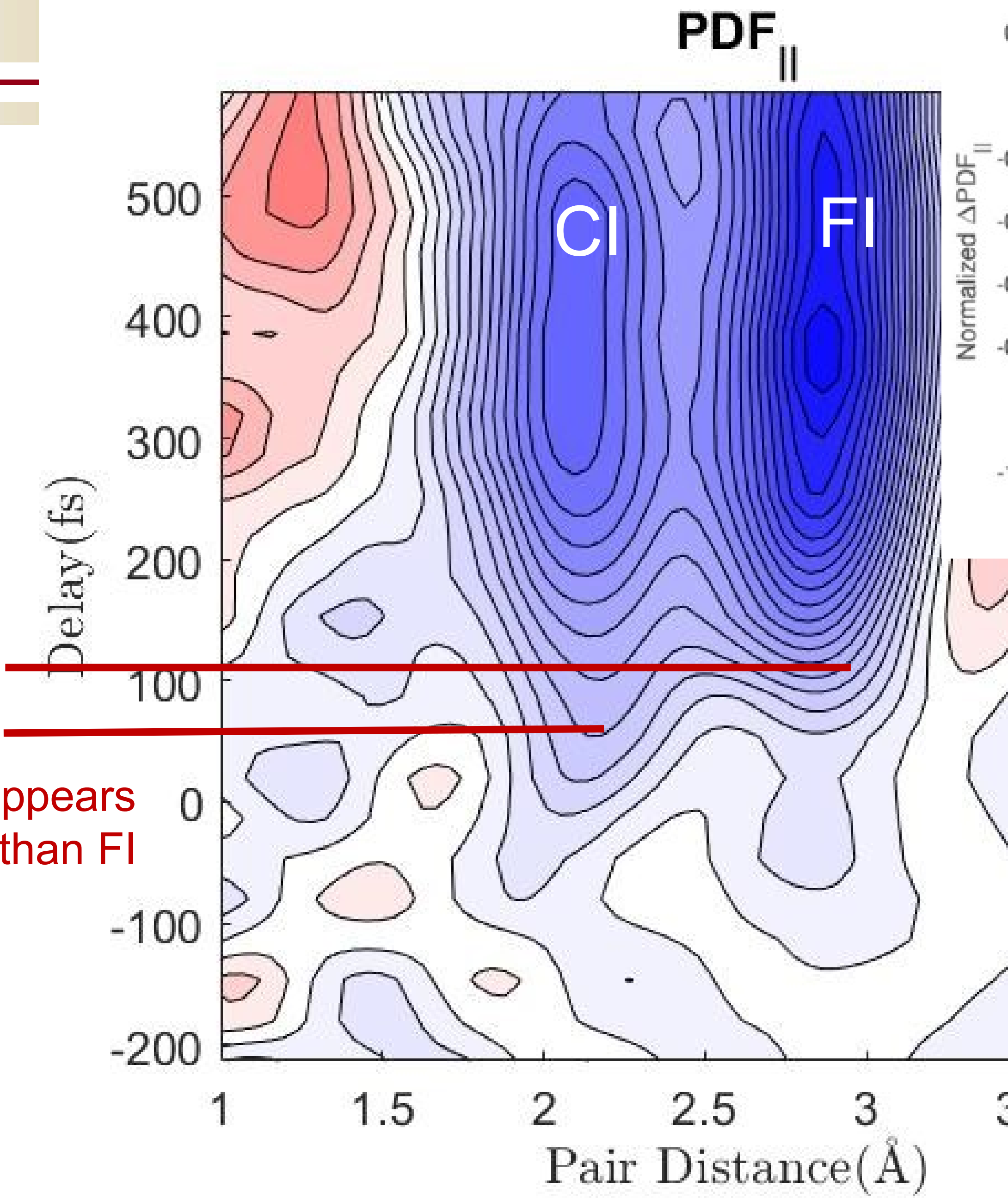
CF_3I Structure Dynamics

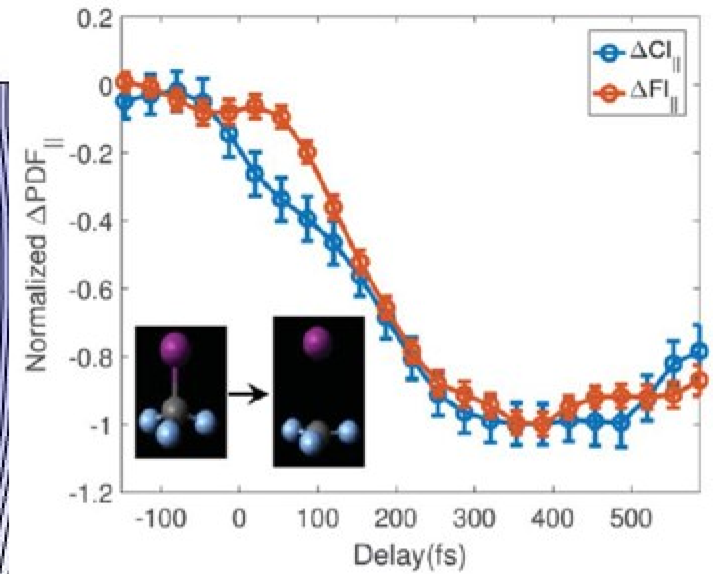


CF_3I Structure Dynamics

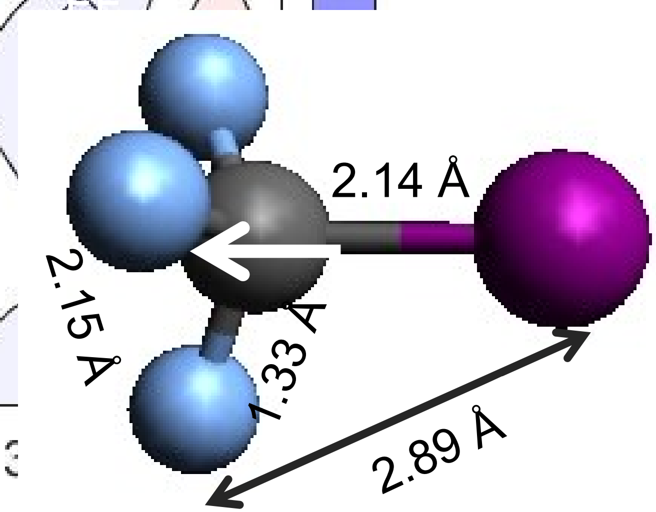


The CI bond bleaches earler than the FI bond



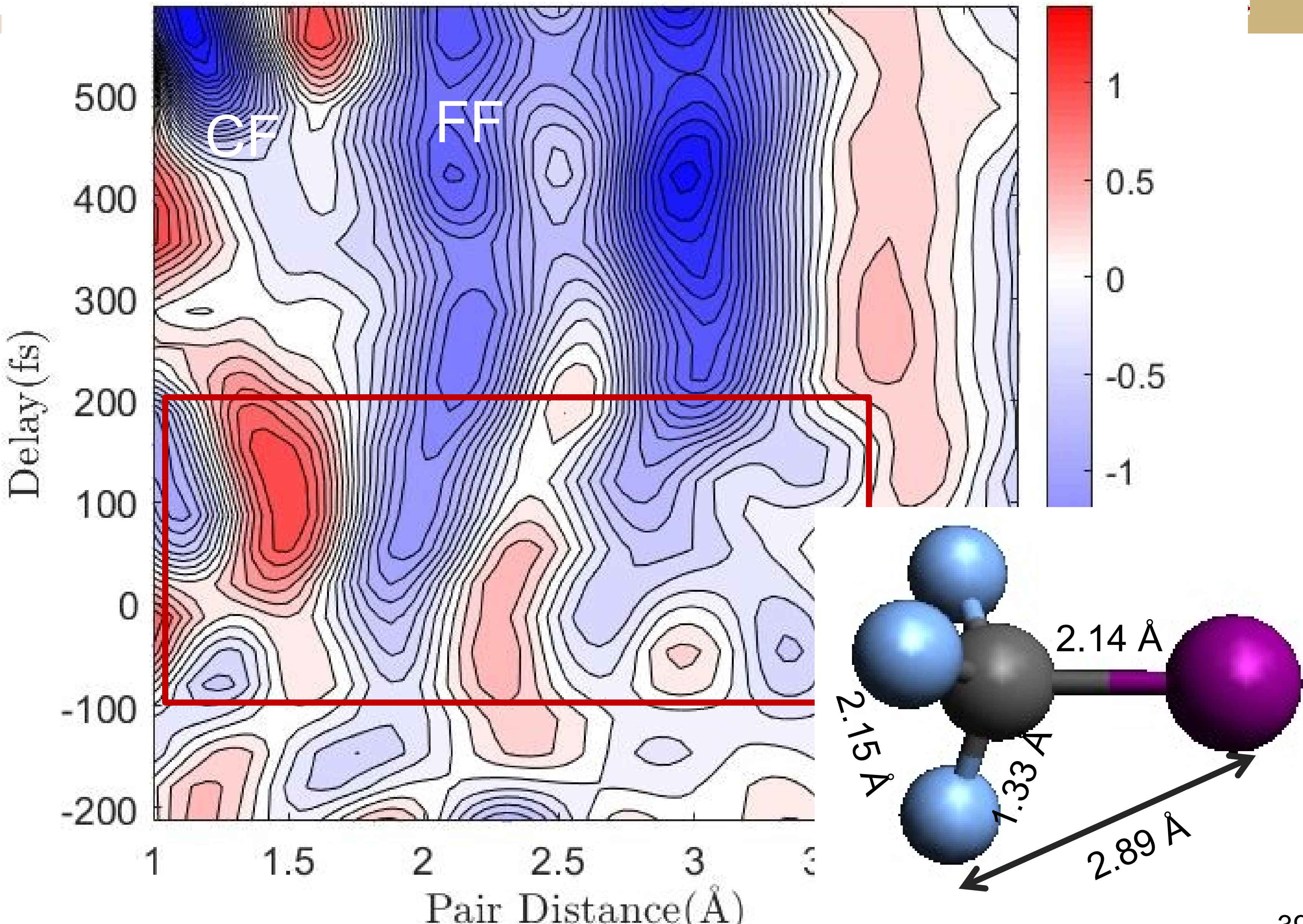


CI disappears
earlier than FI



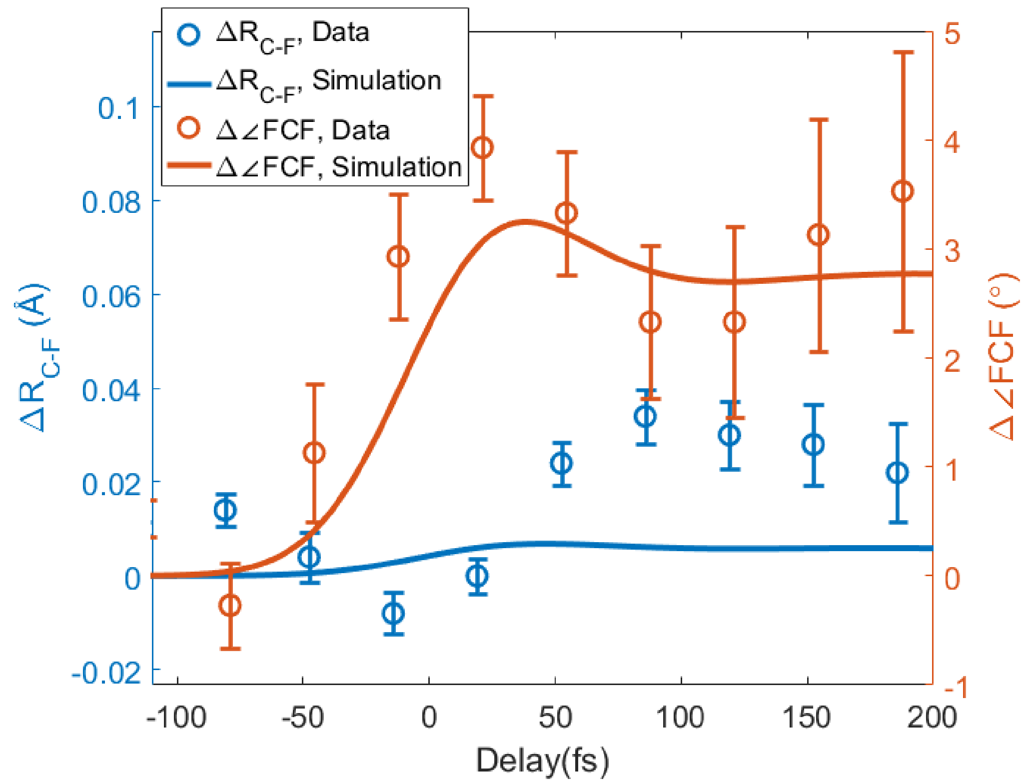
CF_3 group dynamics

∠FCF flattening, followed by a CF lengthening

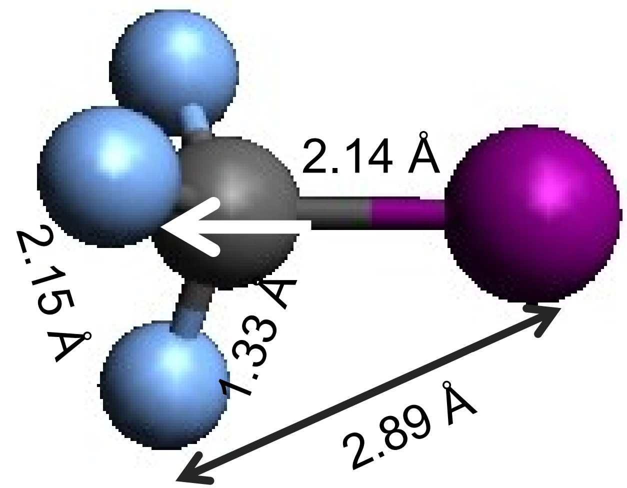


Structure Fitting result

SLAC



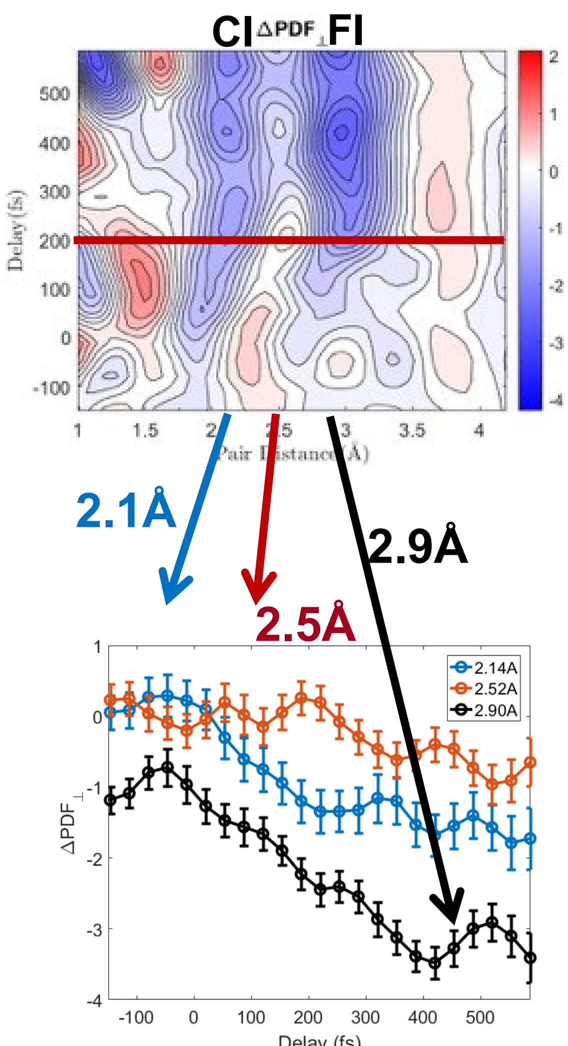
d_{CF} and ∠FCF resolved with 0.01Å and 1° precision!



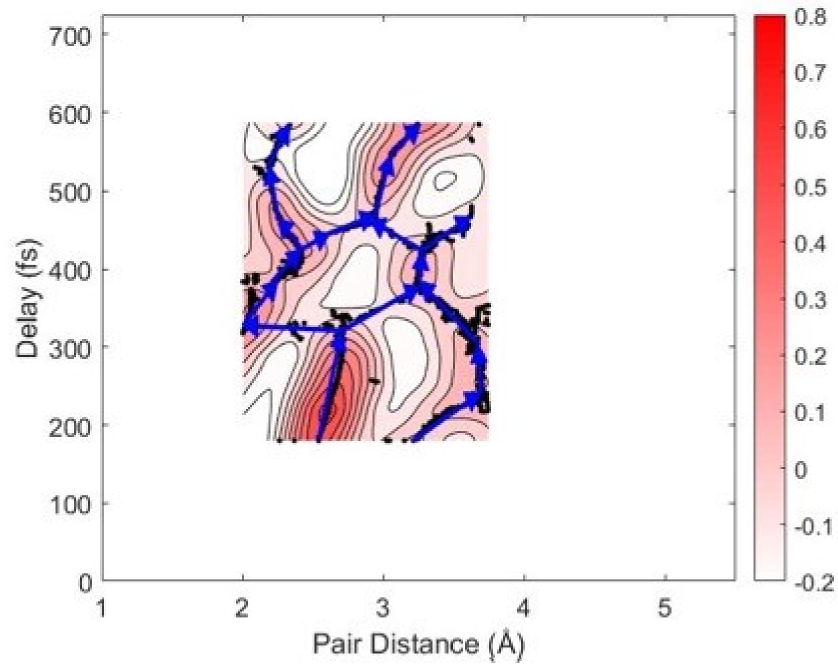
Two Photon Pathway

SLAC

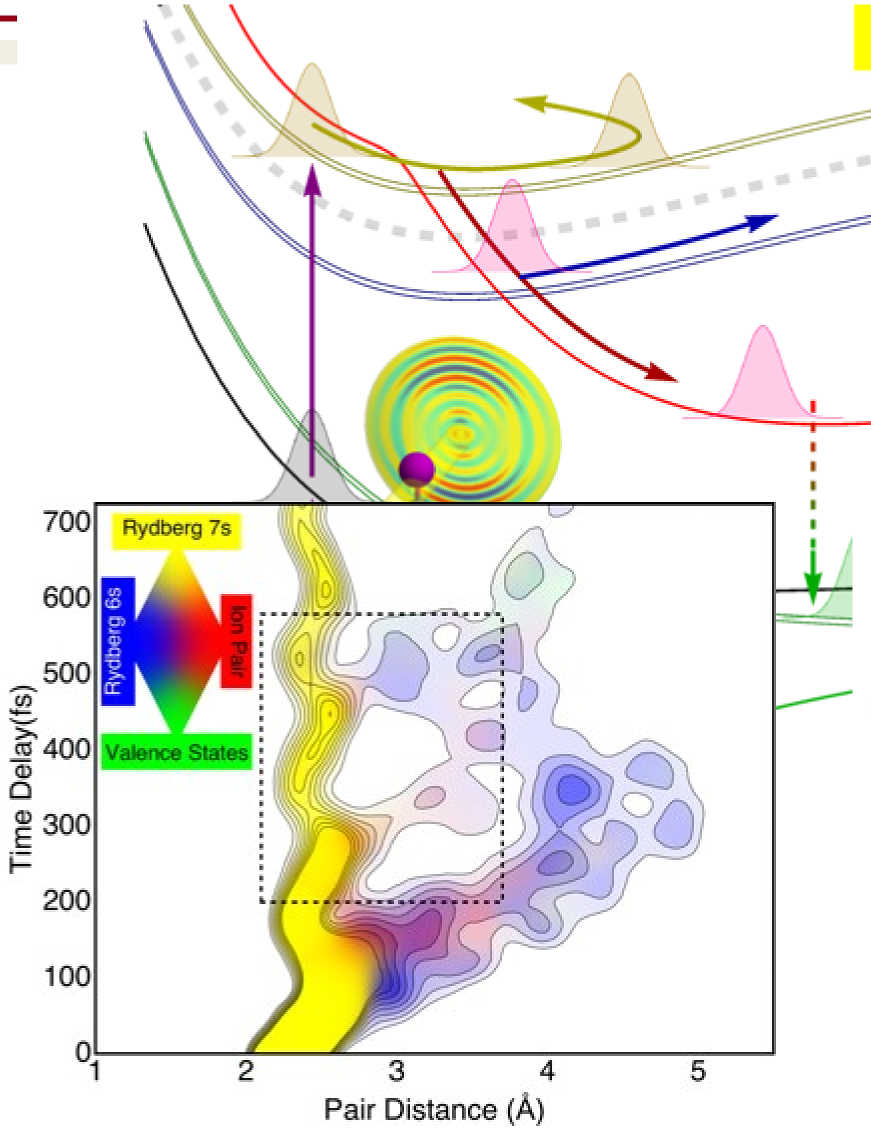
Perpendicular

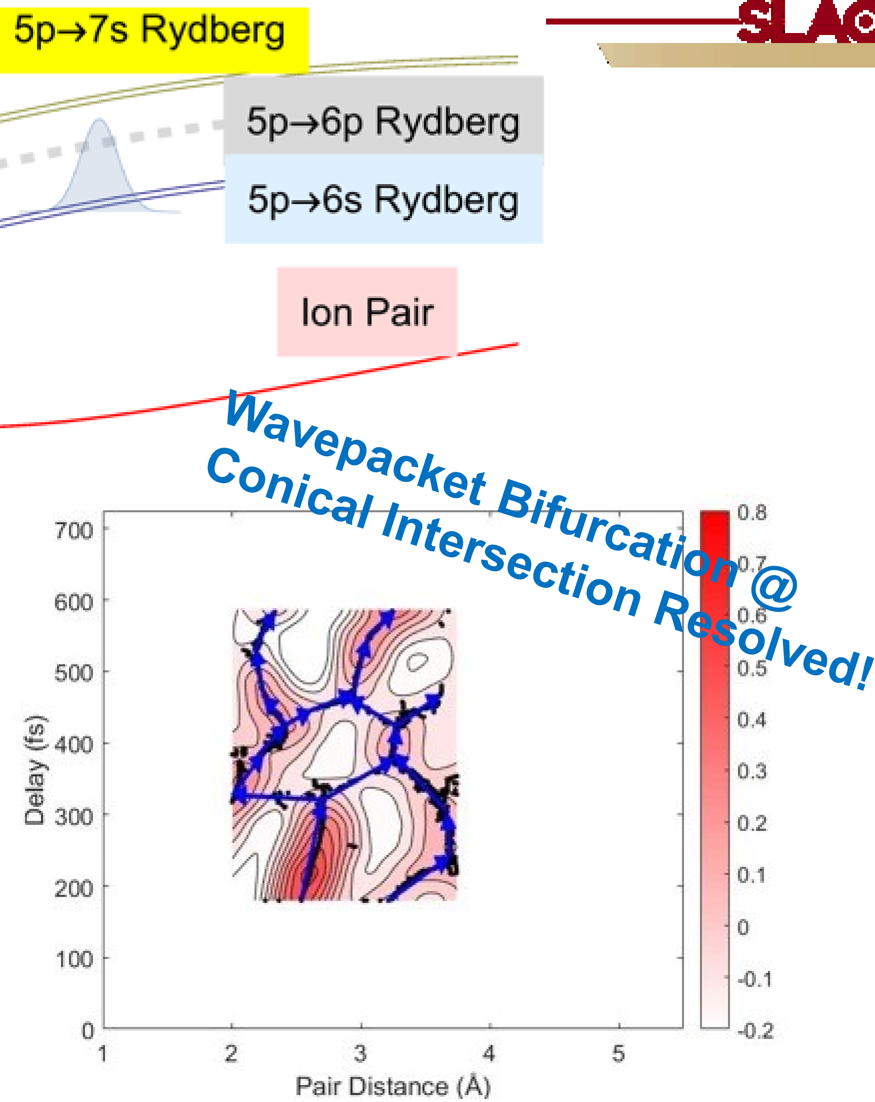


Bleaching signal removed +
Ridge-Detection Algorithm



Two Photon Pathway

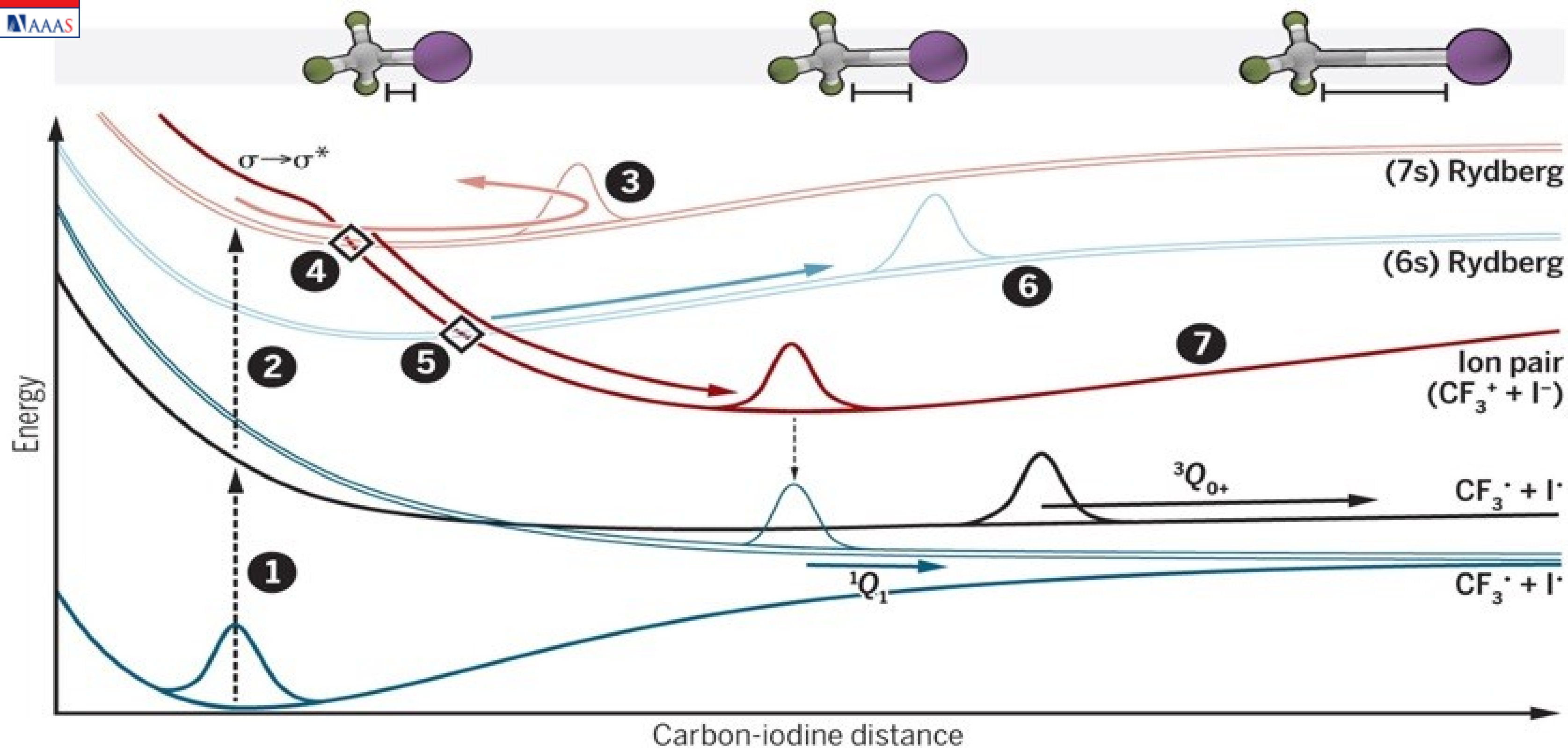




Simulation by Xiaolei Zhu, Martinez group

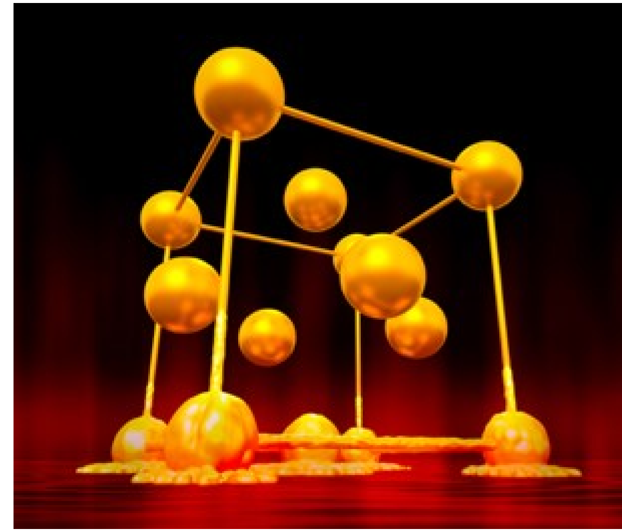
Data

CF_3I Structure Dynamics



1. One-photon excitation
2. Two-photon excitation
3. Excited CF_3I oscillates along a higher-energy Rydberg state.
4. Some molecules cross at the conical intersection to an ion-pair state.
5. Some of the ion-pair population crosses from the ion-pair state to a lower-lying Rydberg state.
6. Population on the Rydberg state undergoes quantum interference.
7. The ion pair loses energy and drops to the radical-pair state.

Science enabled by the high-brightness electron beams

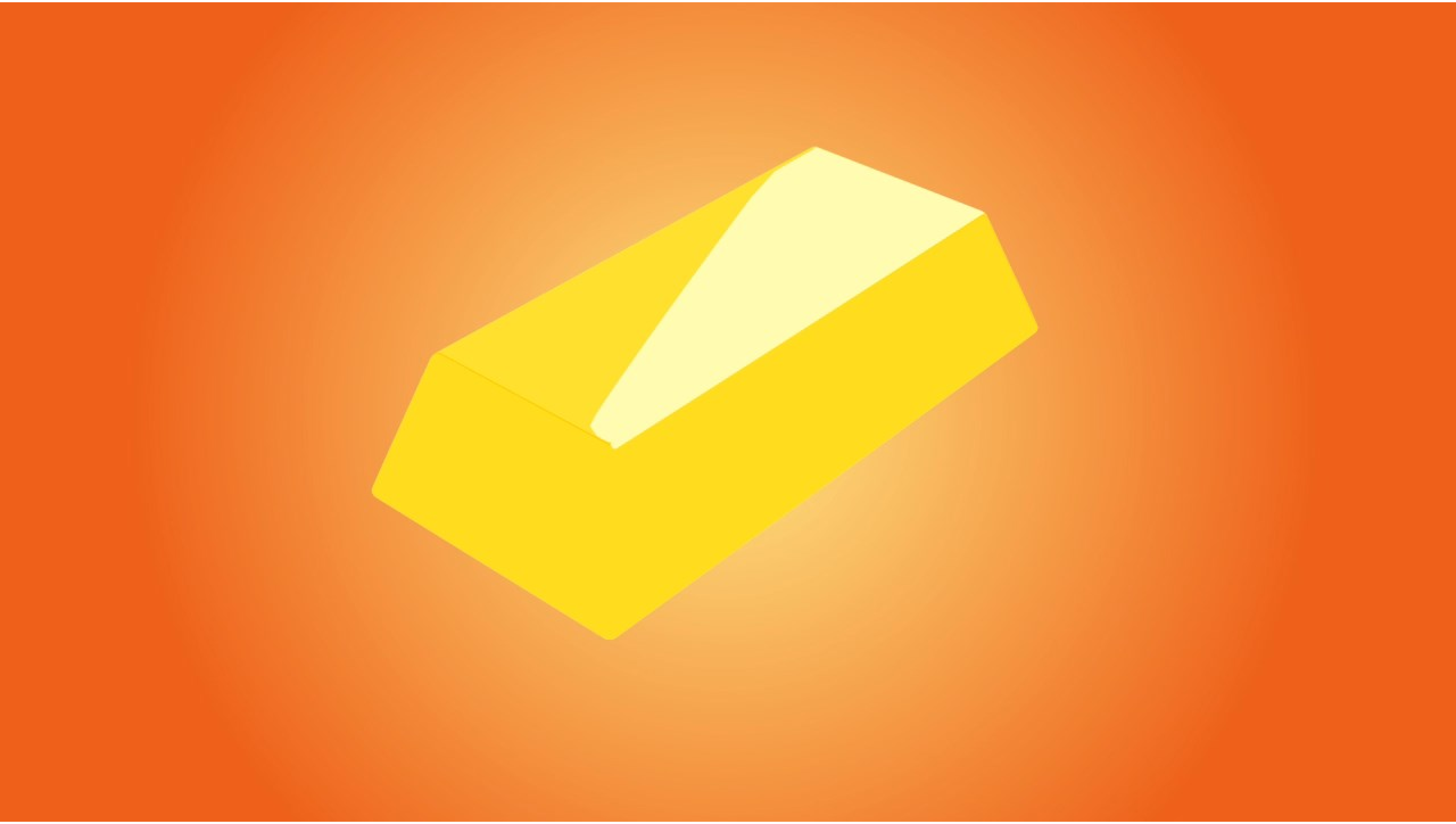


Resolving ultrafast phase transitions
(Science 360 1451–1455 (2018))

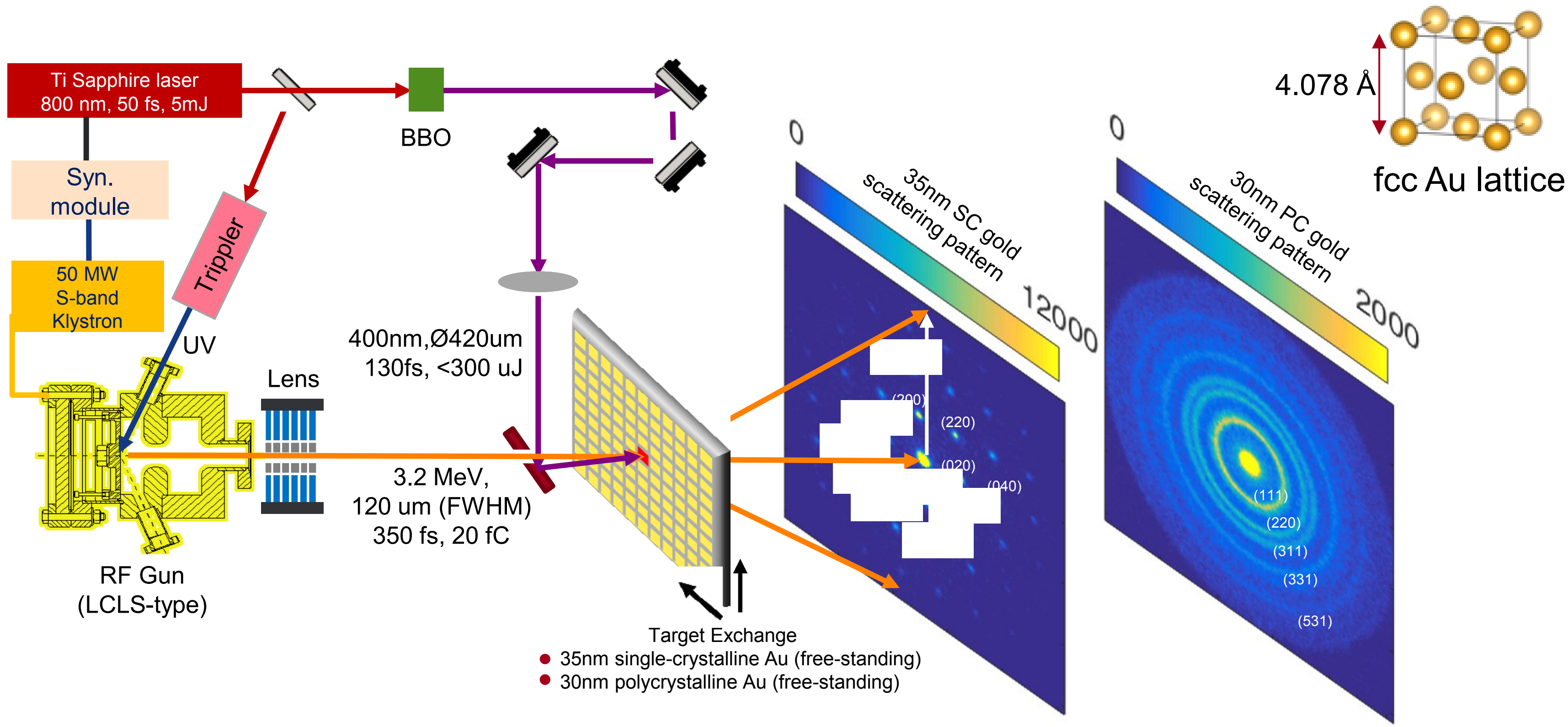
CONDENSED MATTER

Heterogeneous to homogeneous melting transition visualized with ultrafast electron diffraction

M. Z. Mo[1*†], Z. Chen[1†], R. K. Li[1], M. Dunning[1], B. B. L. Witte[1,2], J. K. Baldwin[3], L. B. Fletcher[1], J. B. Kim[1], A. Ng[4], R. Redmer[2], A. H. Reid[1], P. Shekhar[5], X. Z. Shen[1], M. Shen[5], K. Sokolowski-Tinten[6], Y. Y. Tsui[5], Y. Q. Wang[3], Q. Zheng[1], X. J. Wang[1], S. H. Glenzer[1*]

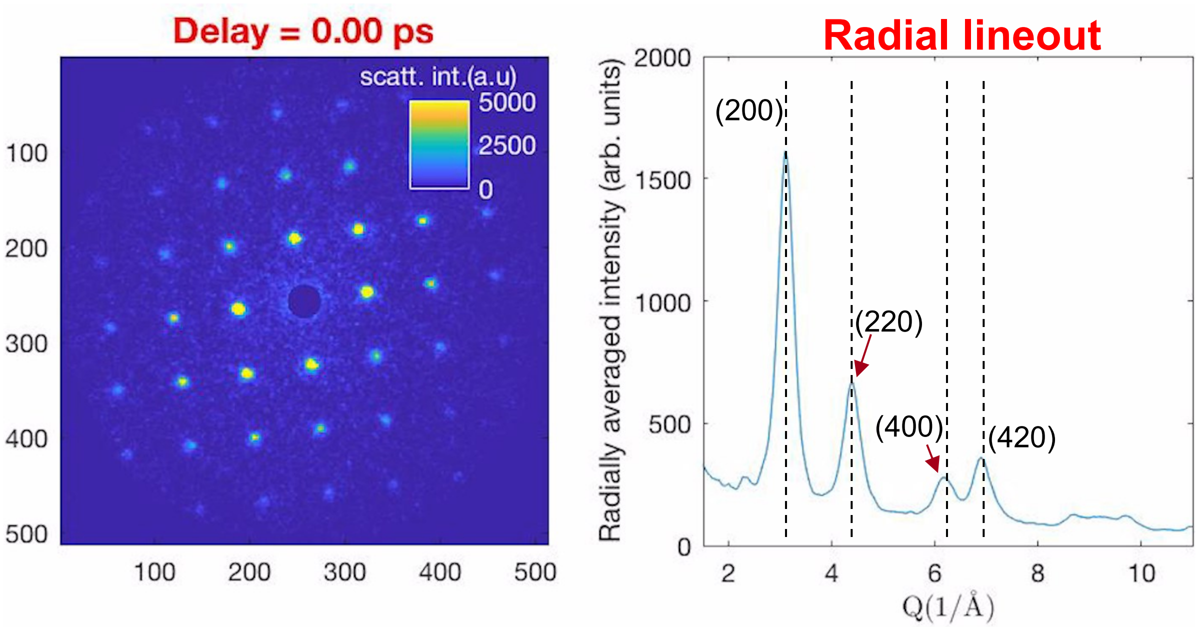


Single-shot MeV-UED to study the structural dynamics of warm dense gold



M.Z. Mo, et al, RSI, **87**, 11D810 (2016)

Ultrafast solid-liquid phase transition of 35nm gold excited with pump fluence of 80 mJ/cm^2 (1.17 MJ/kg)

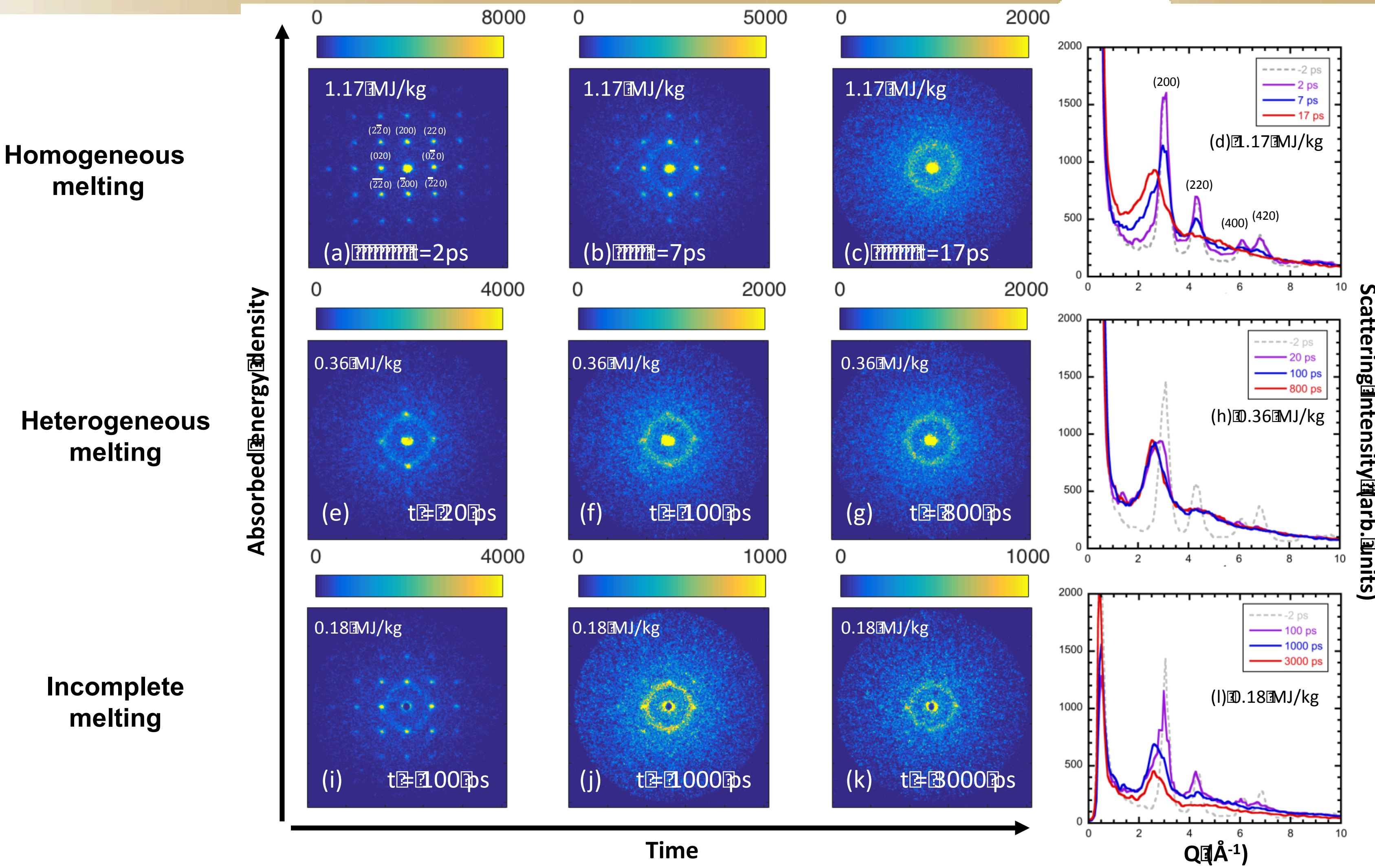


Three obvious features:

- Decay of Laue Diffraction peaks due to thermal heating and structural loss
- Rise of thermal diffuse scattering over the whole spectrum
- Increase of signal from highly disordered liquid structure factor

M. Mo *et al*, Science **360** 1451–1455 (2018))

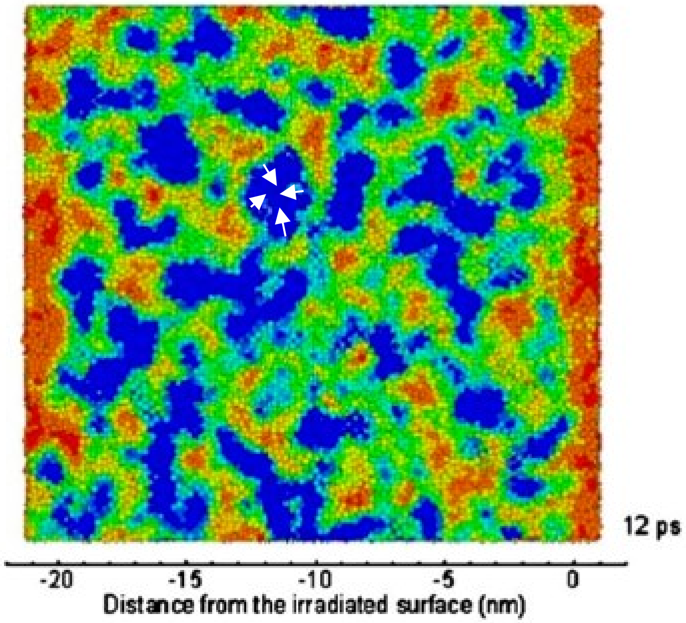
UED has discovered the heterogeneous melting regime that is sensitive to defects and grain boundaries



M. Mo *et al*, Science **360** 1451–1455 (2018))

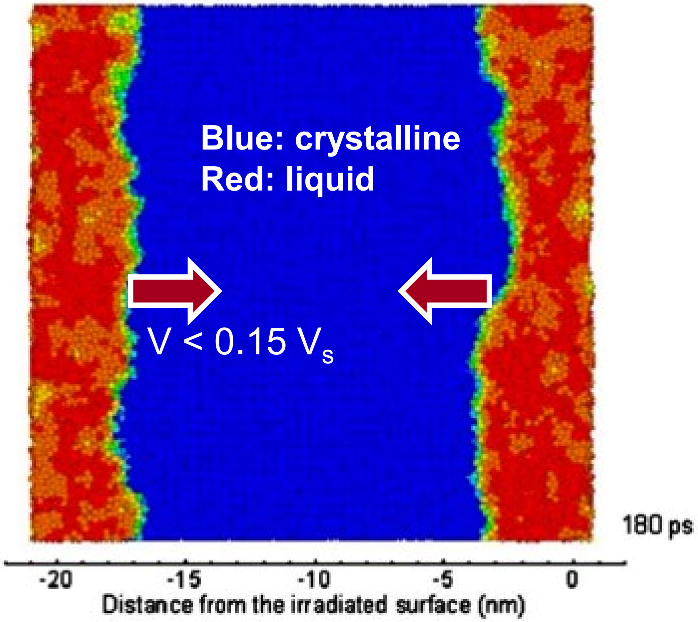
Homogeneous melting occurs catastrophically under strong superheating, whereas heterogeneous melting relies on the melt front propagation with subsonic speed

MD simulated homogenous melting of 20 nm gold excited by fs laser pulse



Nucleates homogeneously

MD simulated heterogeneous melting of 20 nm gold excited by fs laser pulse

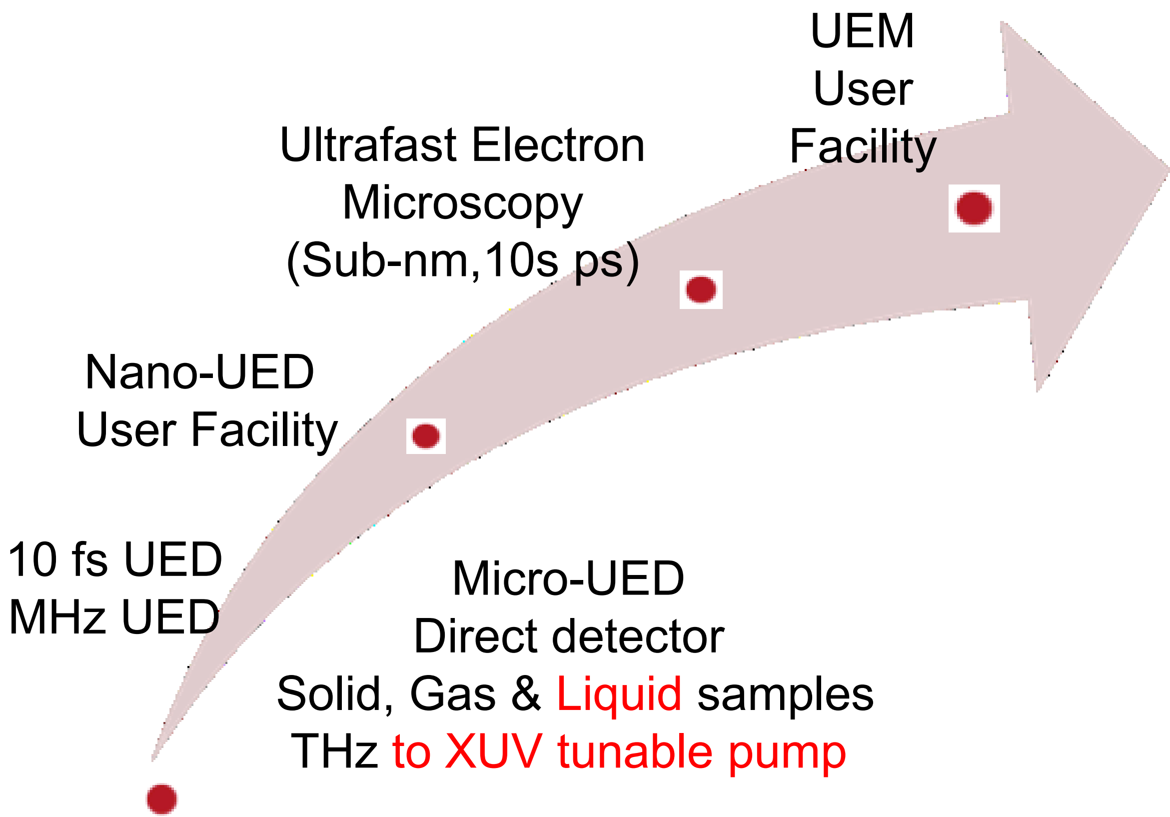


Nucleates from the two free surfaces

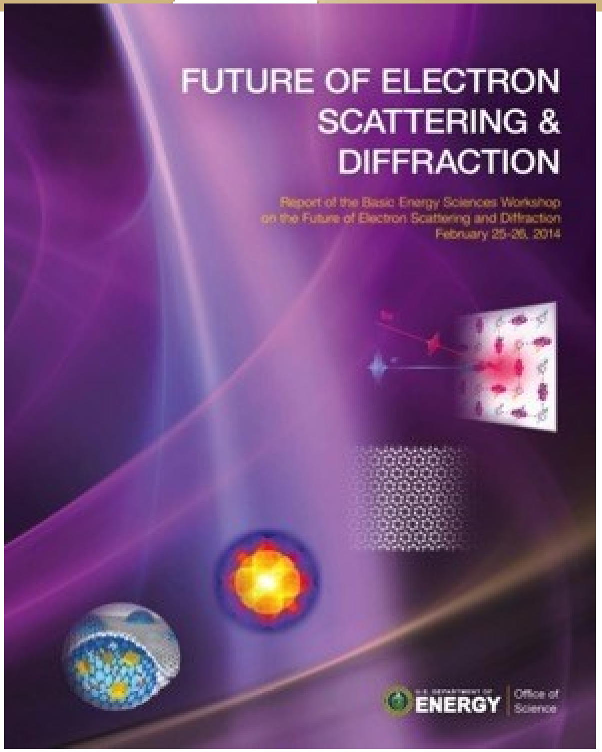
Z. Lin, et al, PRB **73**, 184113 (2006);

M. Mo *et al*, Science **360** 1451–1455 (2018))

SLAC's Vision for Ultrafast Electron Scattering & Microscopy



The first step: MeV Ultrafast Electron Diffraction (UED)



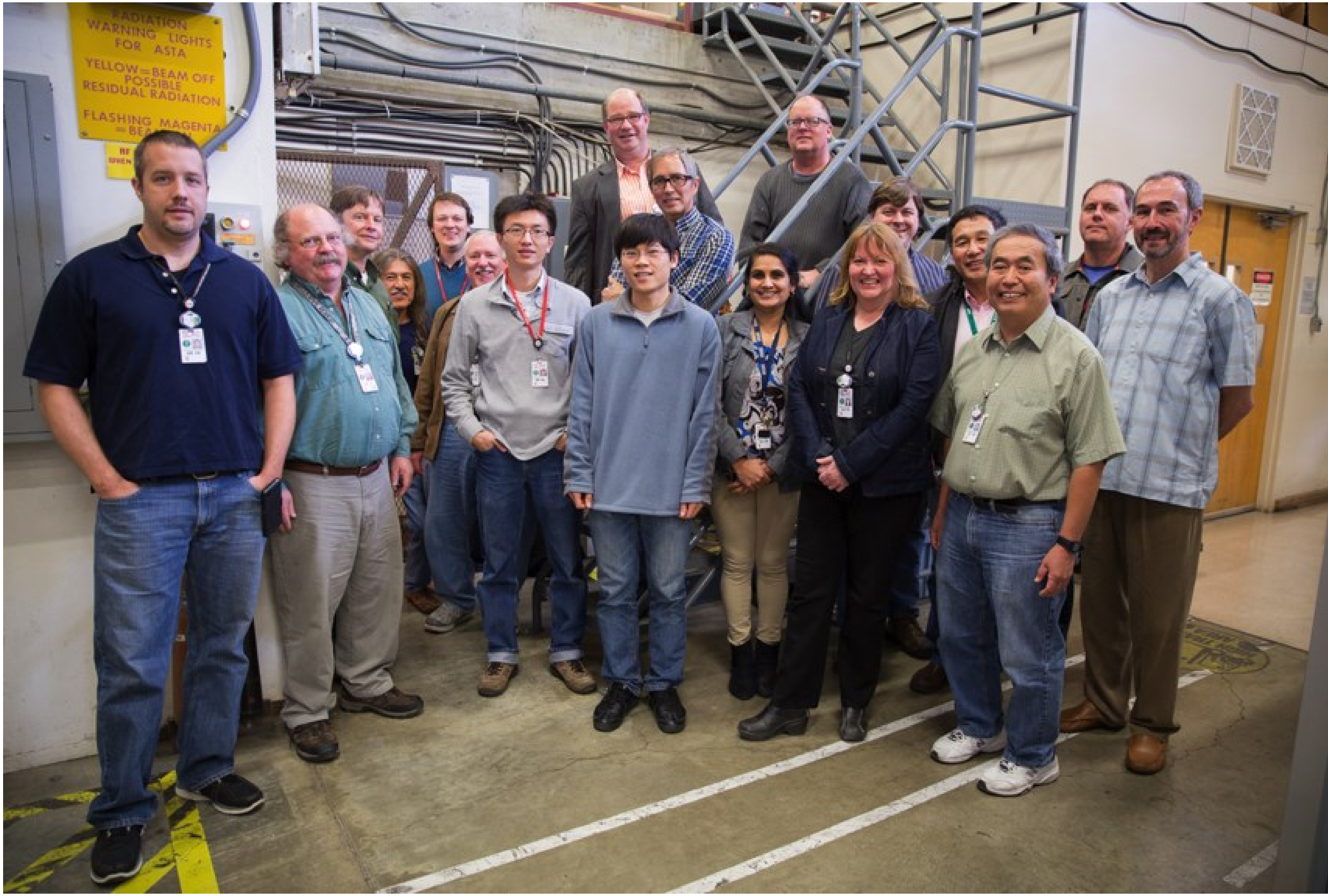
Recommendation: setup ultrafast electron scattering & microscopy facility

Acknowledgement

- SLAC UED program is supported in part by the U.S. Department of Energy (DOE) Office of Basic Energy Sciences Scientific User Facilities Division – Accelerator & Detector R&D Program .

- SLAC UED/UEM Initiative Program Development Funds (SLAC program development and AD program development), and Laboratory Directed Research & Development (LDRD) fund.

- The technical support provided by SLAC Accelerator Directorate, Technology Innovation Directorate, and LCLS is grateful acknowledged.



SLAC's UED/UEM team. From left to right: Theodore Vecchione, Eric Bong, Jeff Corbett, Bobby McKee, Alexander Hume Reid, Perry Anthony, Renkai Li, Carsten Hast, Xiaozhe Shen, Stephen Weathersby, Shanta Condamoor, Keith Jobe, Margery Morse, Garth Brown, Xijie Wang, Charles Yoneda, James Lewandowski, Hermann Dürr., **Not shown: Ryan Coffee, Juan Cruz, Juan, John Eichner, Nick Hartmann , Josef Frisch, Bo Hong, Erik Jongewaard, Justin May, Doug McCormick, Minh Nguyen, Dentell Reed, Daniel Van Winkle & Juhao Wu**

Acknowledgement

Gas UED Experimental Team

SLAC MeV UED Team: **Jie Yang**, Renkai Li, Xiaozhe Shen, etc.

Stanford Pulse Institute: Thomas Wolf, James Cryan,

University of Nebraska-Lincoln: Martin Centurion, Matt Robinson

University of Postdam: Markus Guehr

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Theoretical Support

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