Advanced Imaging with the XFEL and Potential of Attosecond Coherent Diffractive Imaging

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The FUture of SEeded free Electron lasers (FUSEE) Workshop
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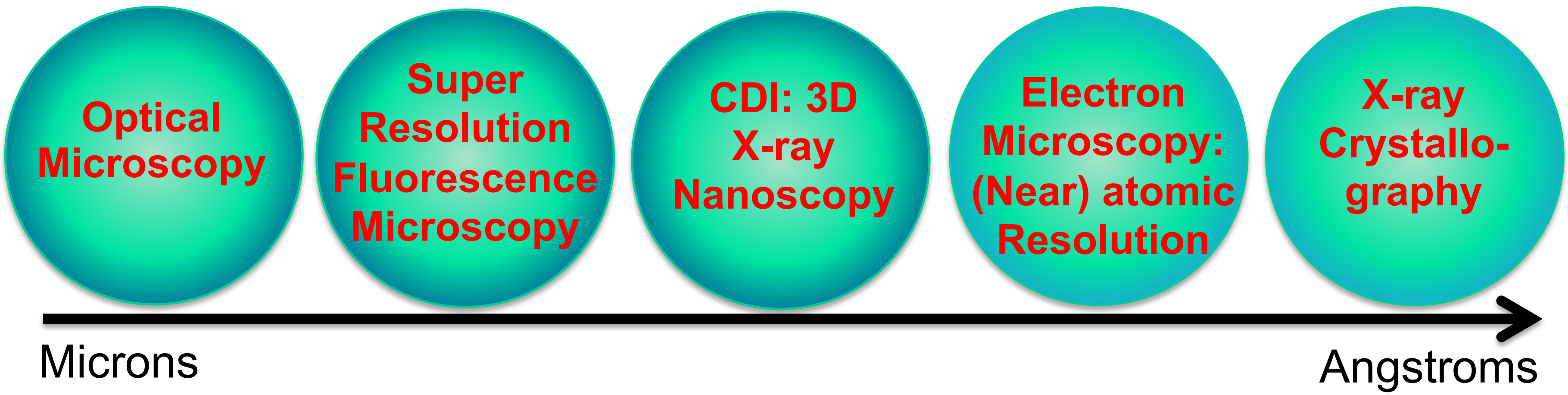
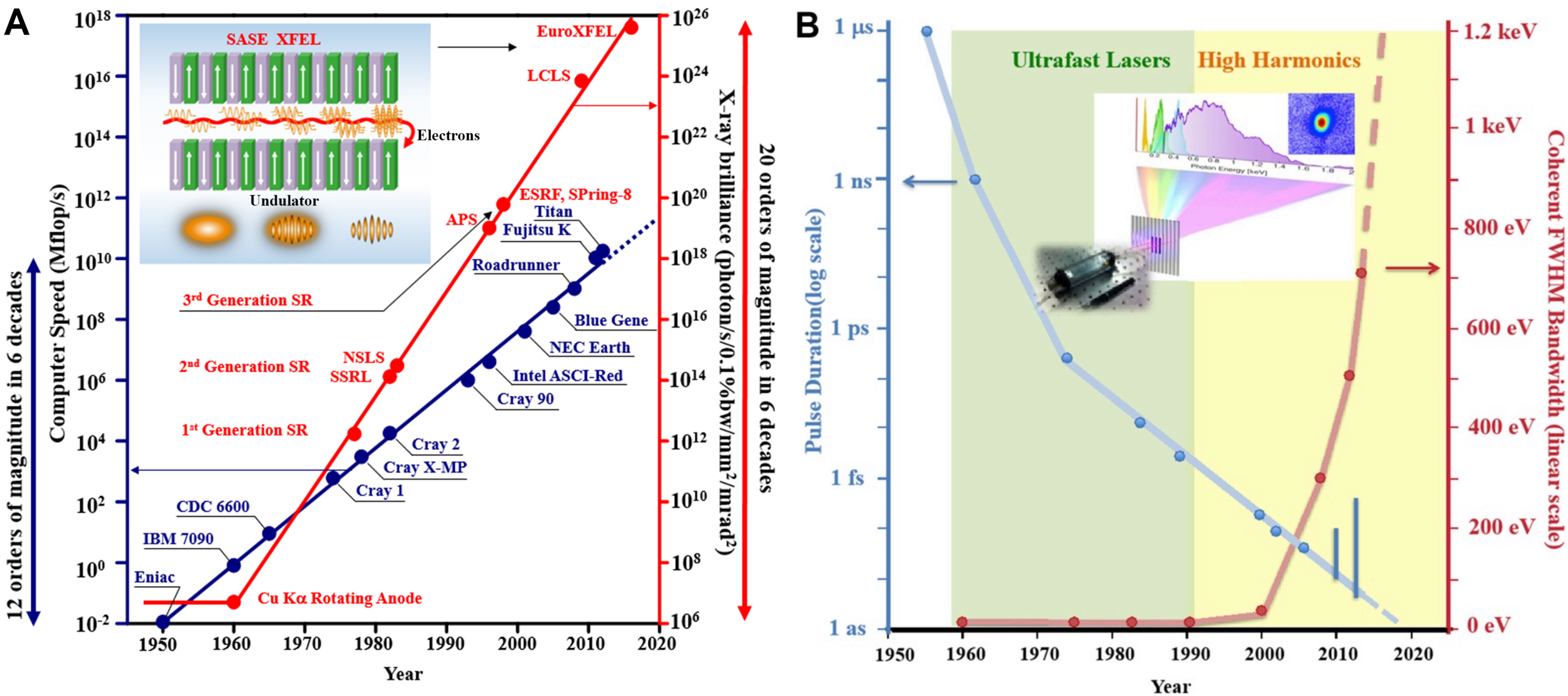
Revolutions in Imaging and Structure Determination



Time scales: minutes to femtoseconds

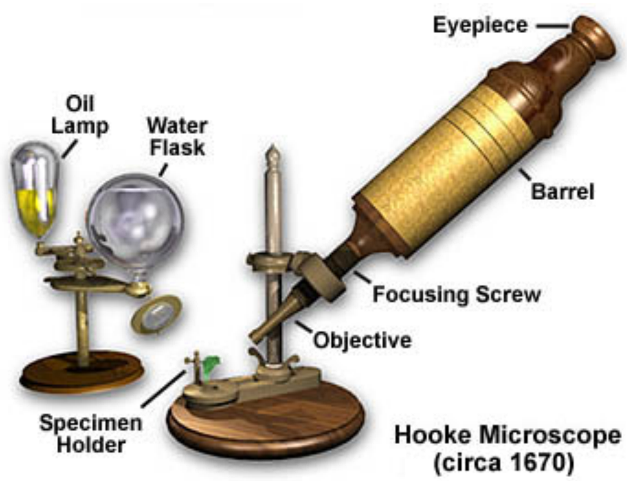
- **Brilliant X-ray sources (such as X-ray free electron lasers and advanced synchrotrons) and aberration-corrected electron microscopy**
- **Powerful imaging methods such as super-resolution fluorescence microscopy, cryo-electron microscopy, optical tweezers and coherent diffractive imaging (CDI)**
- **High dynamic range detectors with single photon or electron counting**
- **Advanced algorithms, big data handling, fast computers and machine leaning**

Breakthrough in Coherent X-ray Sources

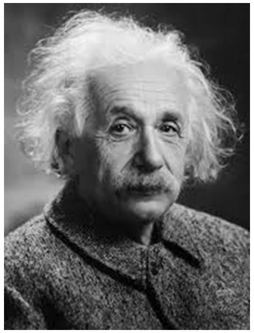


Miao, Ishikawa, Robinson & Murnane, *Science* **348**, 530–535 (2015). (Review)

Coherent Diffractive Imaging: From Lens-Based Microscopy to Lensless Microscopy



The first compound microscope consisting of an objective lens and an eyepiece was built in Europe in the 17th century. Over the last more than three centuries, lens-based microscopy such as optical, phase-contrast, fluorescence, confocal, super-resolution and electron microscopy has played an important role in the evolution of modern science and technology.

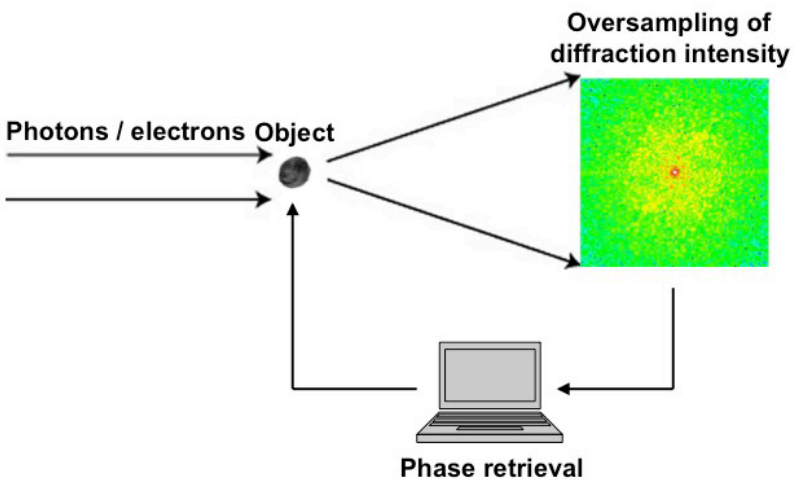
(a) 

 **(b)**

Fourier magnitudes of **(a)** + Fourier phases of **(b)**

Fourier magnitudes of **(b)** + Fourier phases of **(a)**

Coherent Diffractive Imaging:
From Lens-Based Microscopy to Lensless Microscopy



A new type of microscopy based on the Young's double slit experiment

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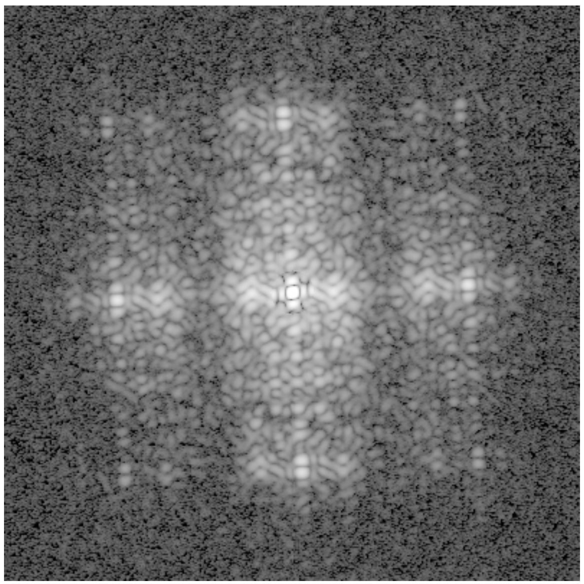
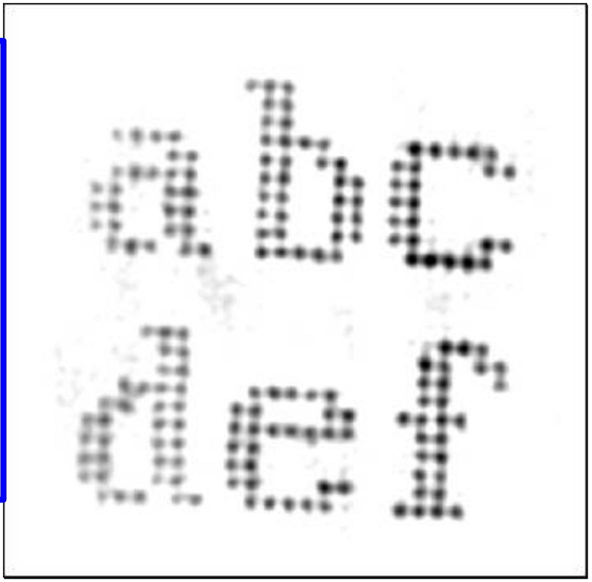


Coherent X-ray diffraction pattern

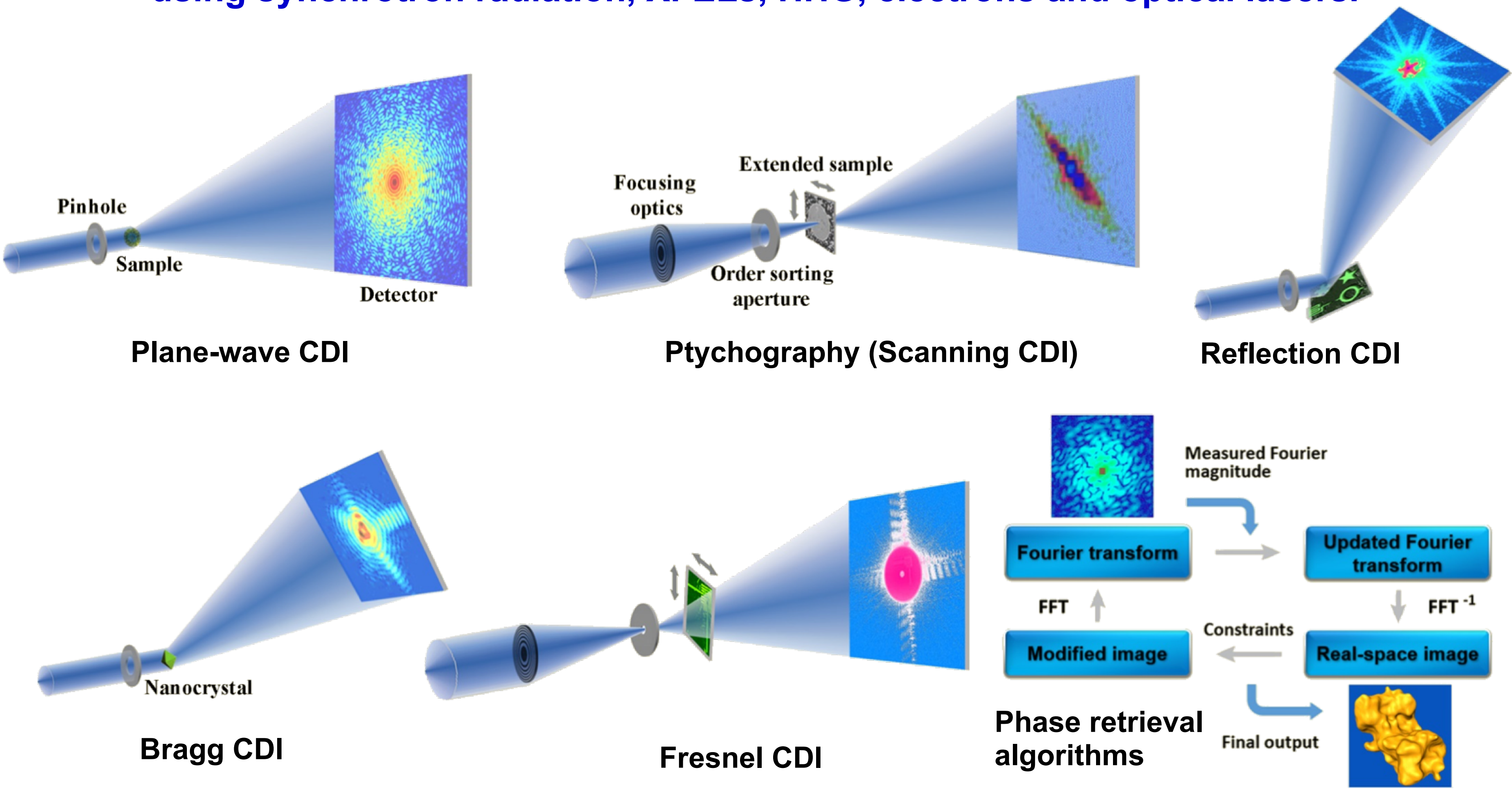
First experimental demonstration of CDI: replacing the physical lenses with coherent illumination and computational algorithms (lensless imaging or computational microscopy)



Miao et al., *Nature* **400**, 342-344 (1999).

Coherent Diffractive Imaging Methods

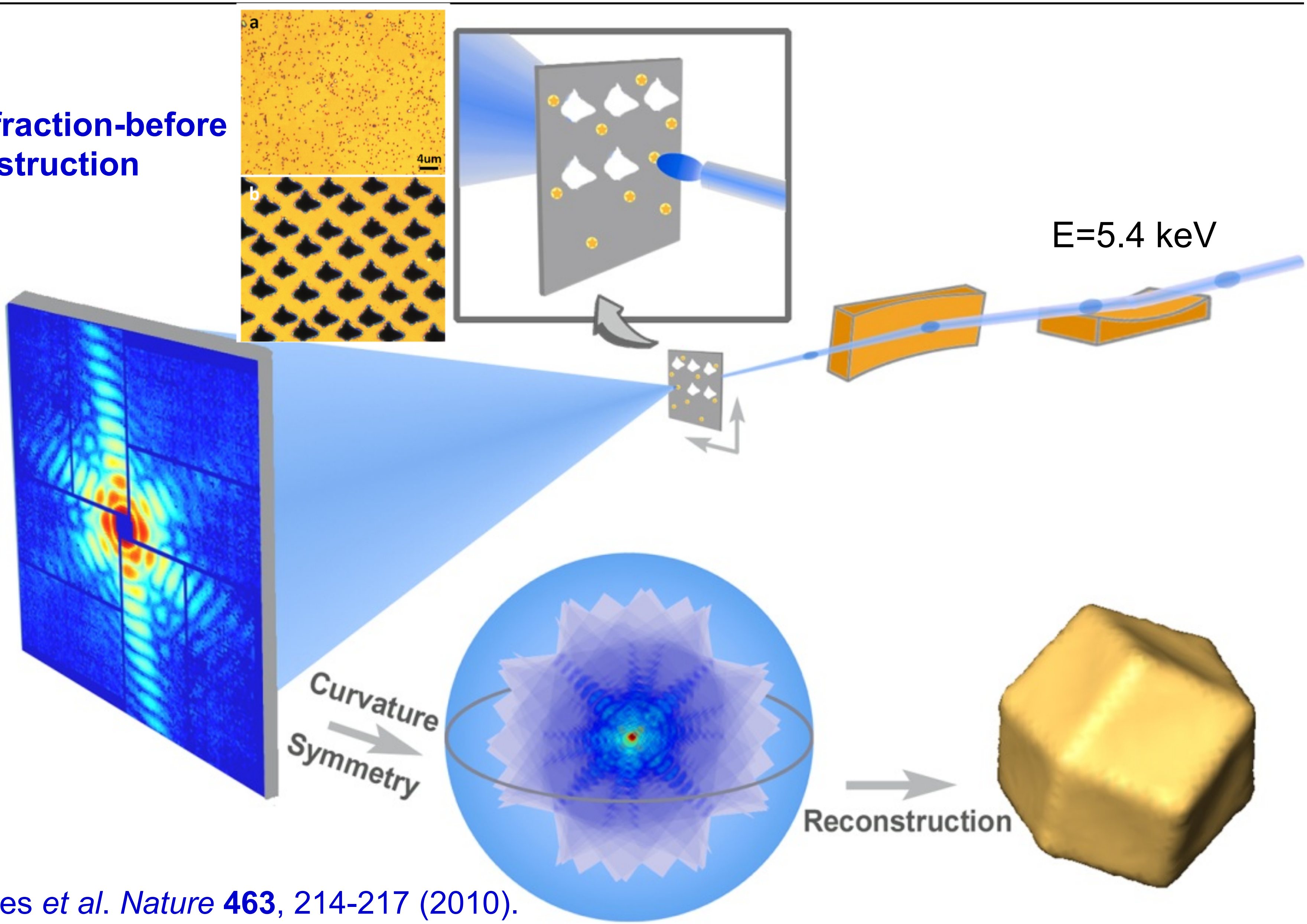
CDI methods have been applied to the physical and biological sciences using synchrotron radiation, XFELs, HHG, electrons and optical lasers.



Miao, Ishikawa, Robinson & Murnane, *Science* **348**, 530–535 (2015). (Review)

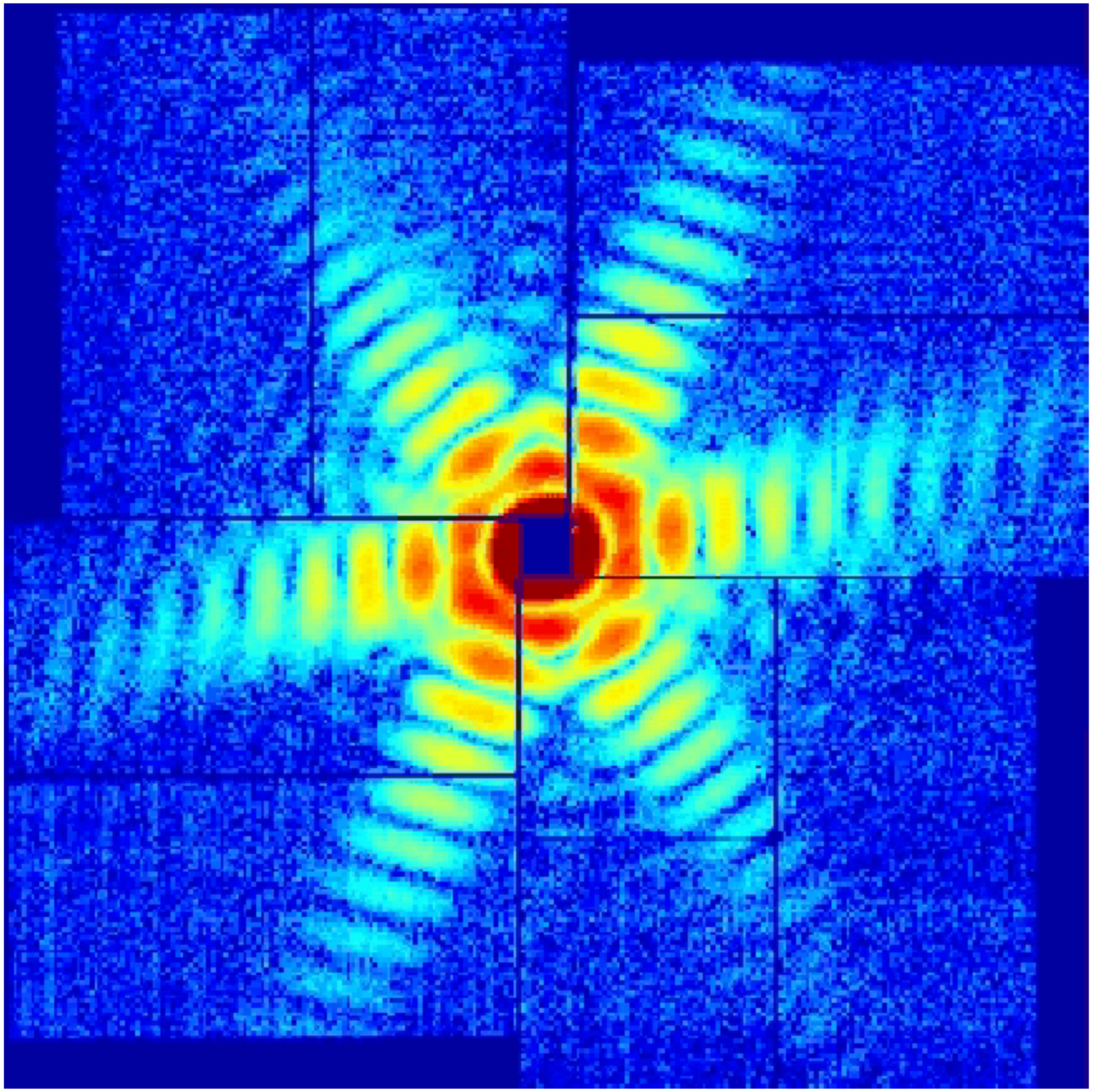
Single-Shot 3D Imaging Experiment with the XFEL

Diffraction-before -destruction

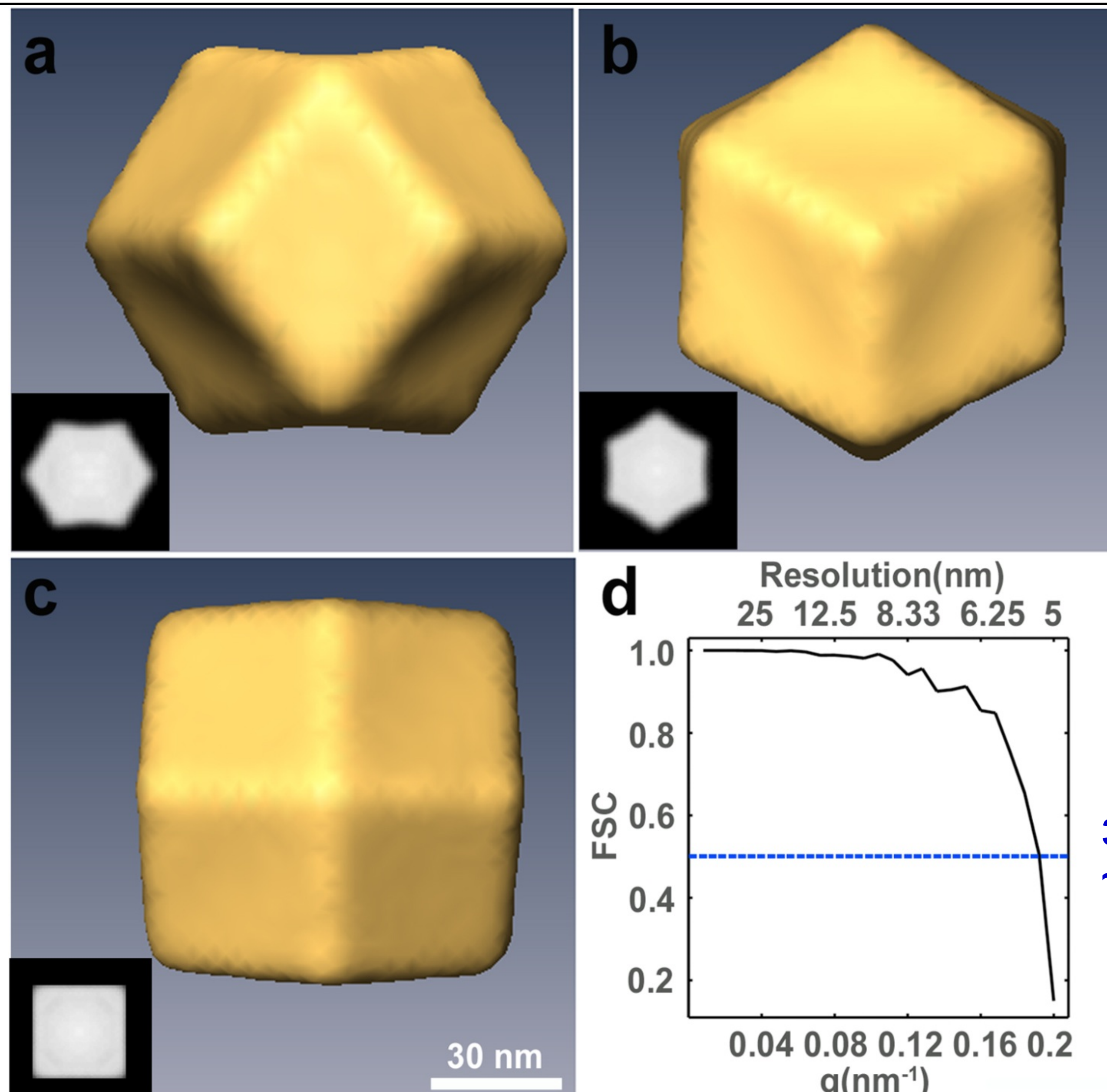


Raines *et al*. *Nature* **463**, 214-217 (2010).

High Quality Single-Shot Diffraction Patterns

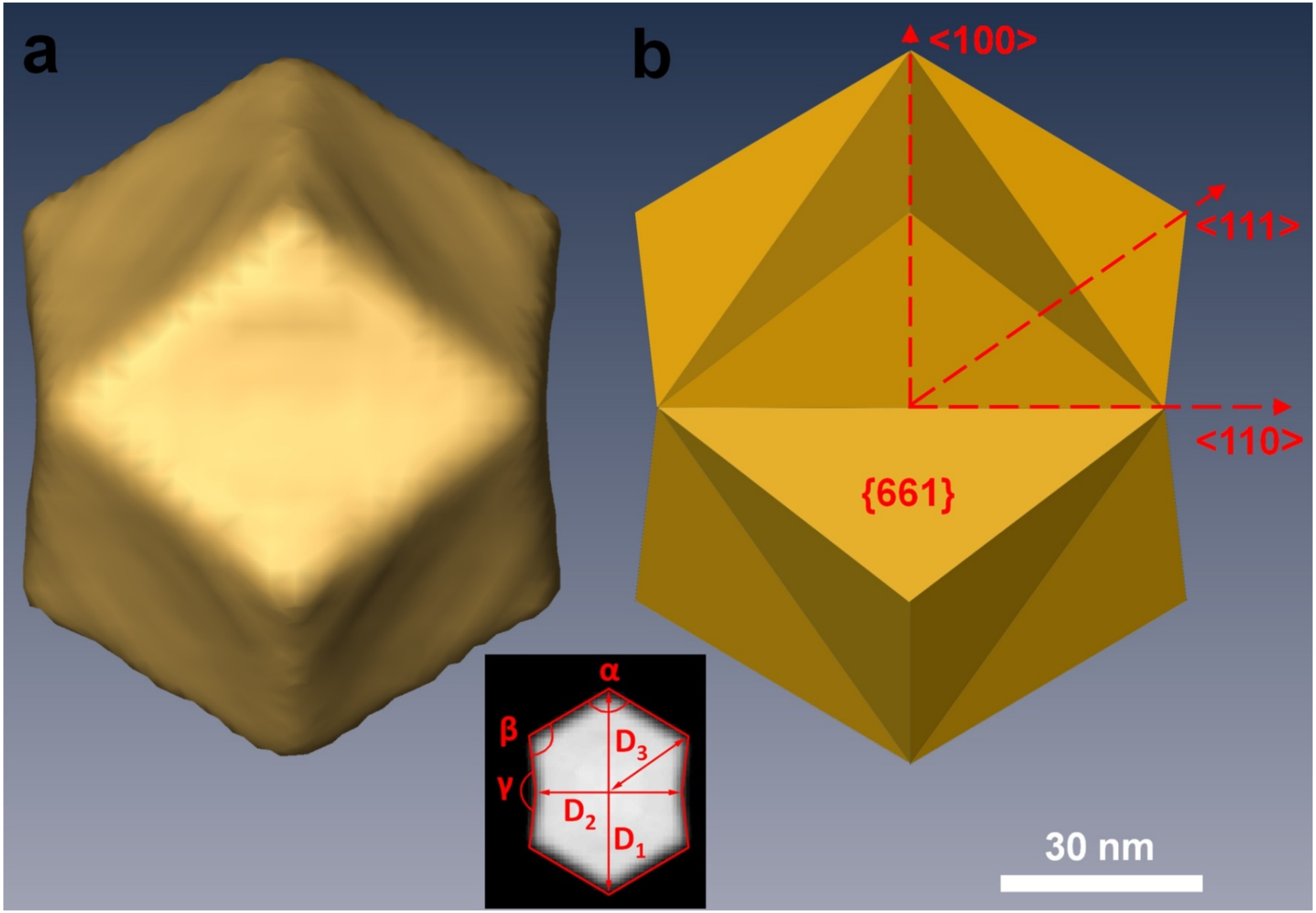


3D Reconstruction of a Single-Shot Diffraction Pattern



3D spatial resolution: ~5.5 nm in ~10 fs.

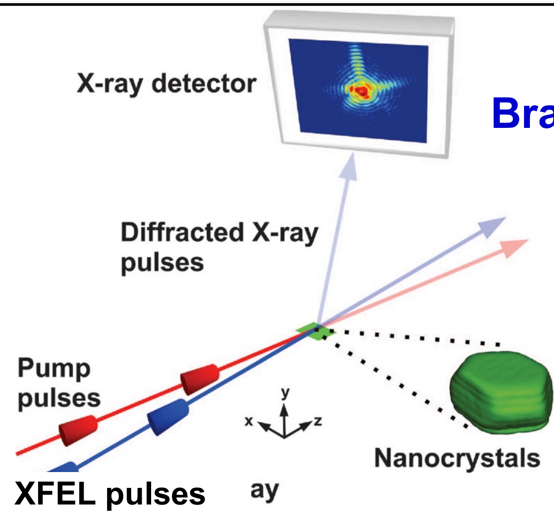
A 3D Model of the Trisoctahedral Au Nanocrystal Obtained from the Single-Shot 3D Reconstruction



α = 119.3° β = 113.4° γ = 166.1° D_1 = 102.6 nm D_2 = 72.3 nm D_3 = 48.5 nm

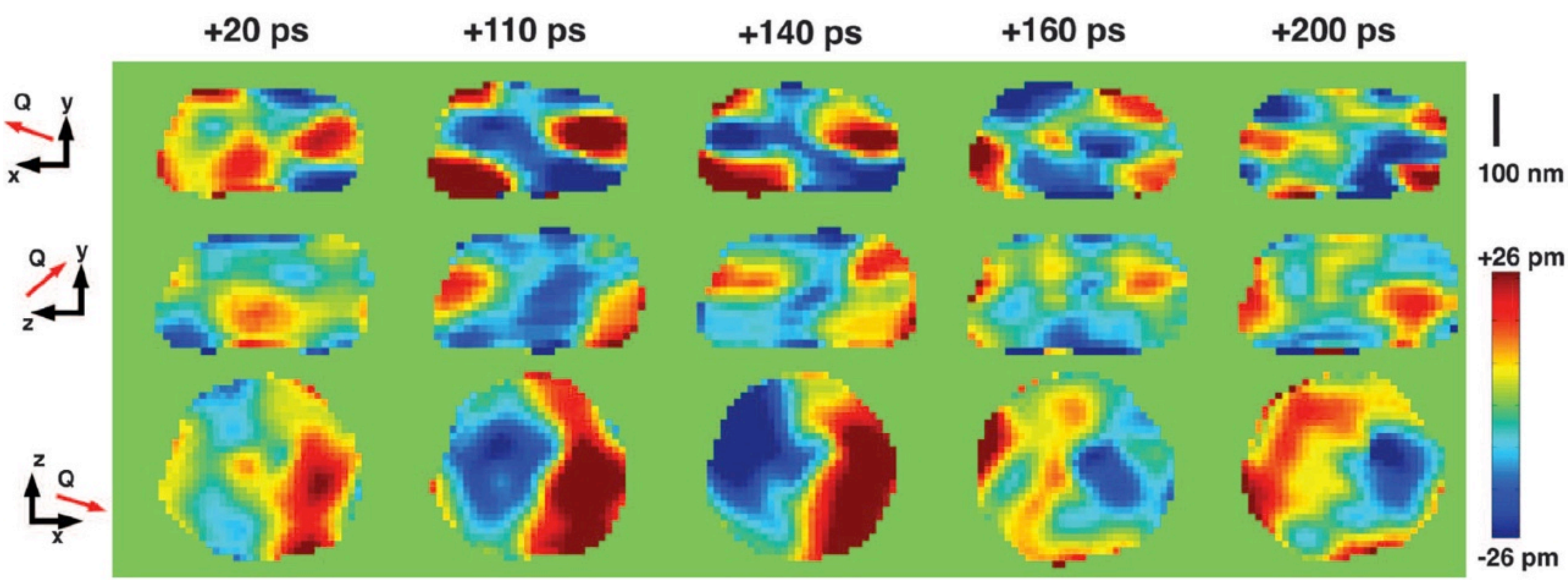
Xu *et al*., *Nature Commun.* **5**, 4061 (2014); Pryor *et al*., *Sci. Rep*. **8**,8284 (2018).

3D Imaging of Lattice Dynamics in Individual Gold Nanocrystals



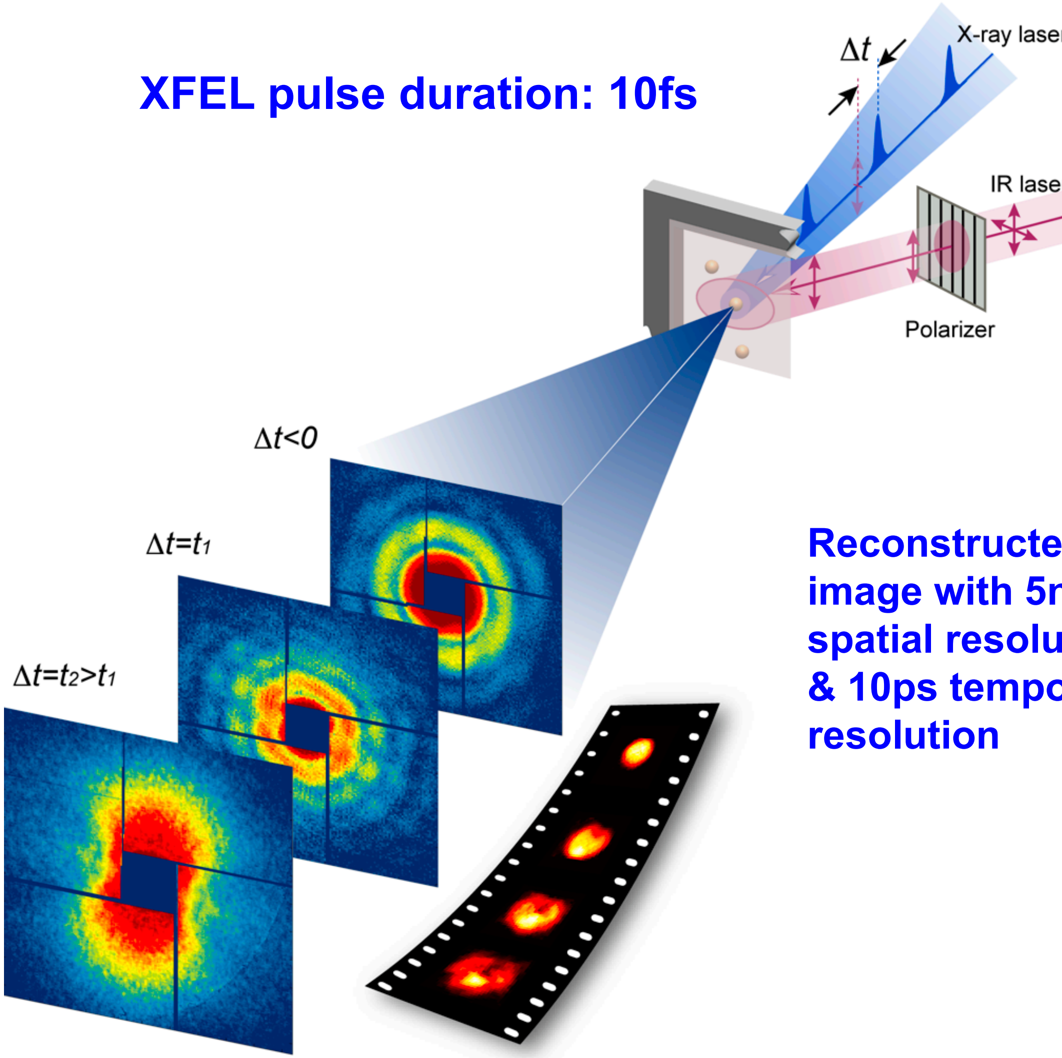
Bragg CDI

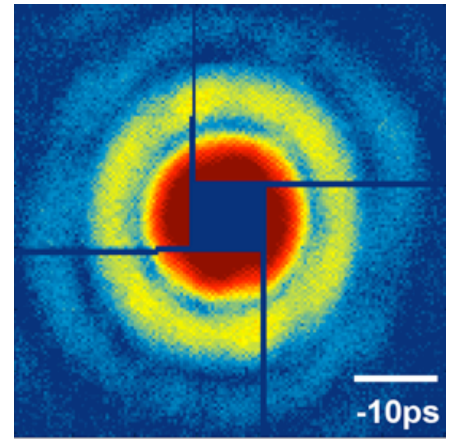
Clark *et al*, *Science* **341**, 56-59 (2013).



Time-Resolved CDI with 5-nm-Spatial Resolution and 10-ps-Temporal Resolution

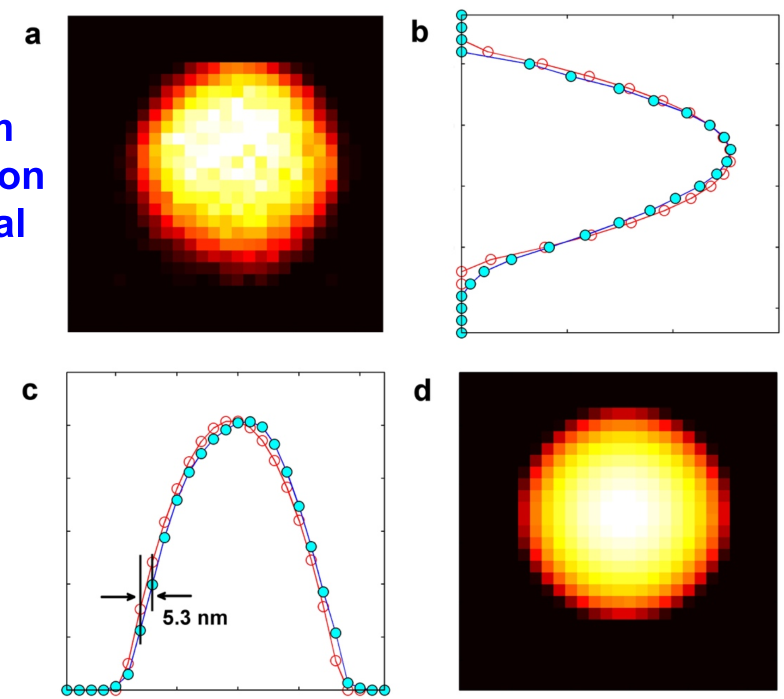
XFEL pulse duration: 10fs





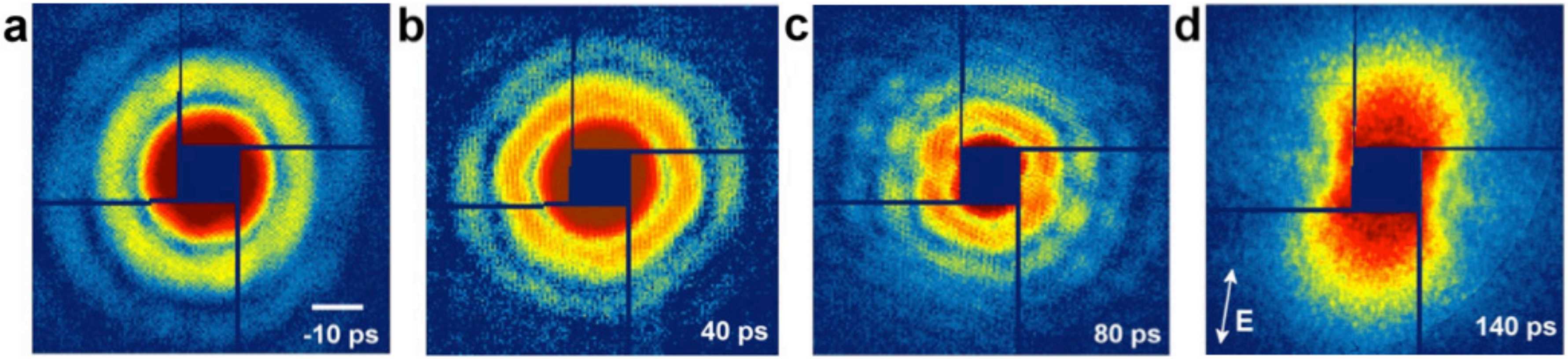
Single-shot diffraction Pattern of a 72 nm Au nanoparticle

Reconstructed image with 5nm spatial resolution & 10ps temporal resolution

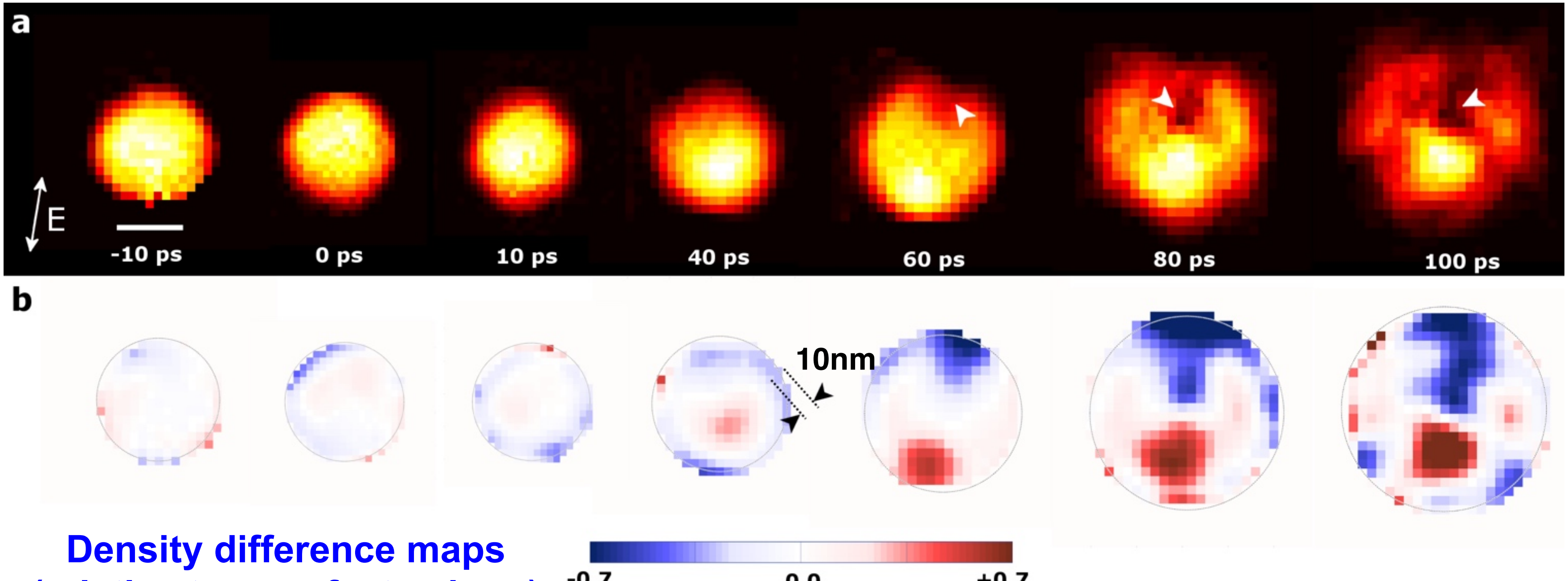


Direct Observation of Irreversible Melting

Single-shot diffraction patterns with polarization-dependent anisotropic distortion

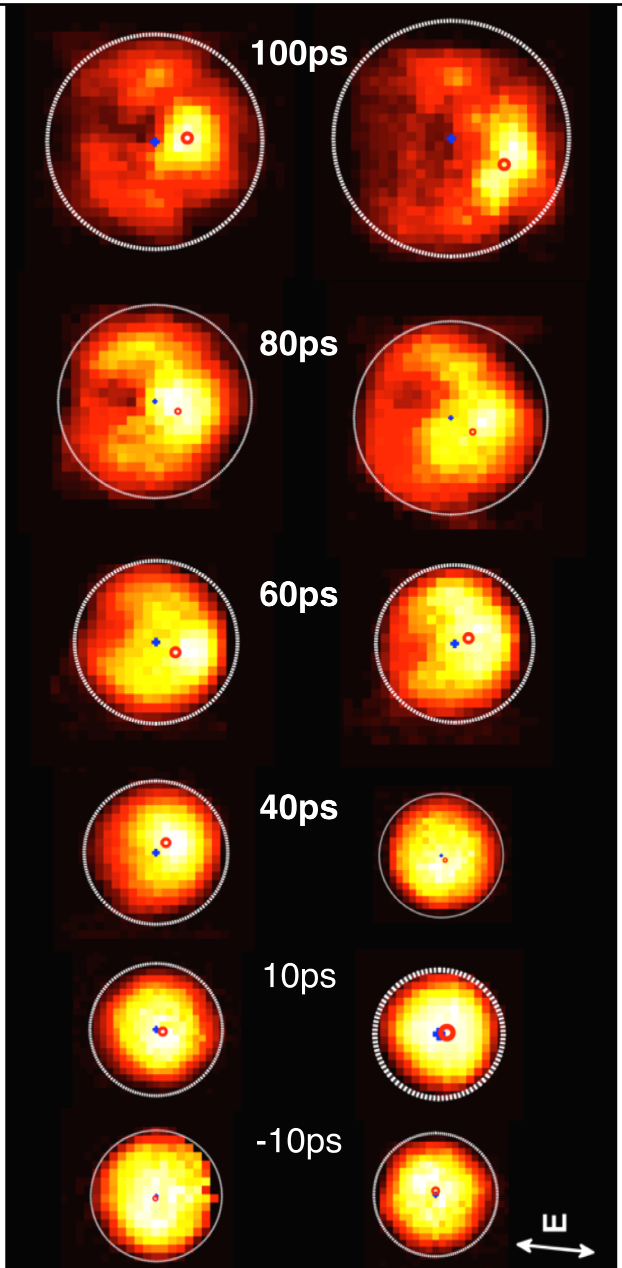


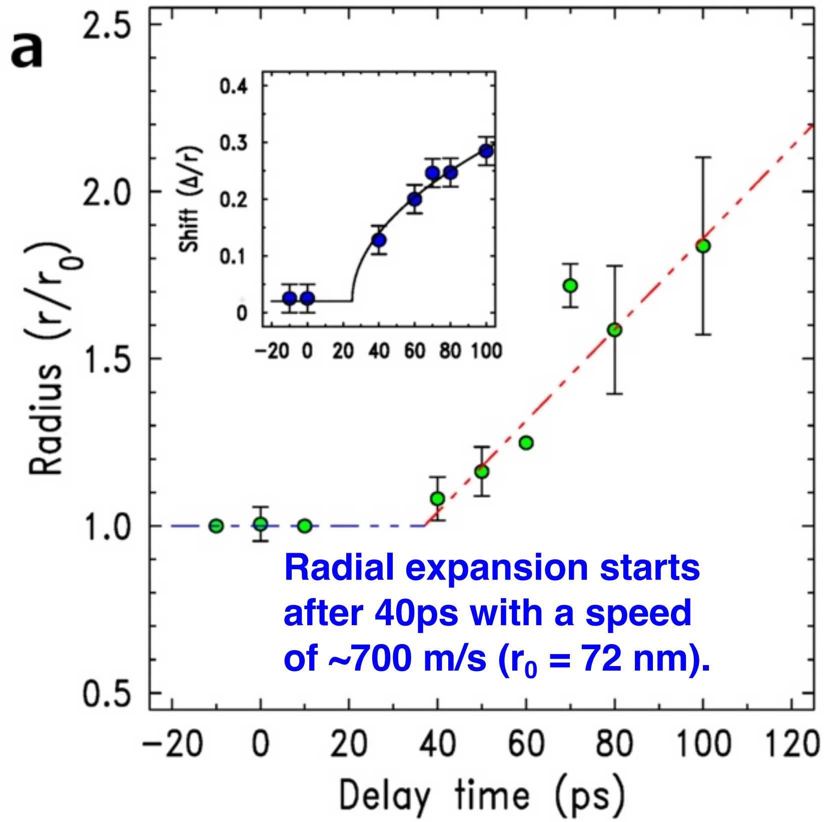
Reconstructed images



Density difference maps (relative to a perfect sphere)

Polarization-Induced Anisotropic Melting





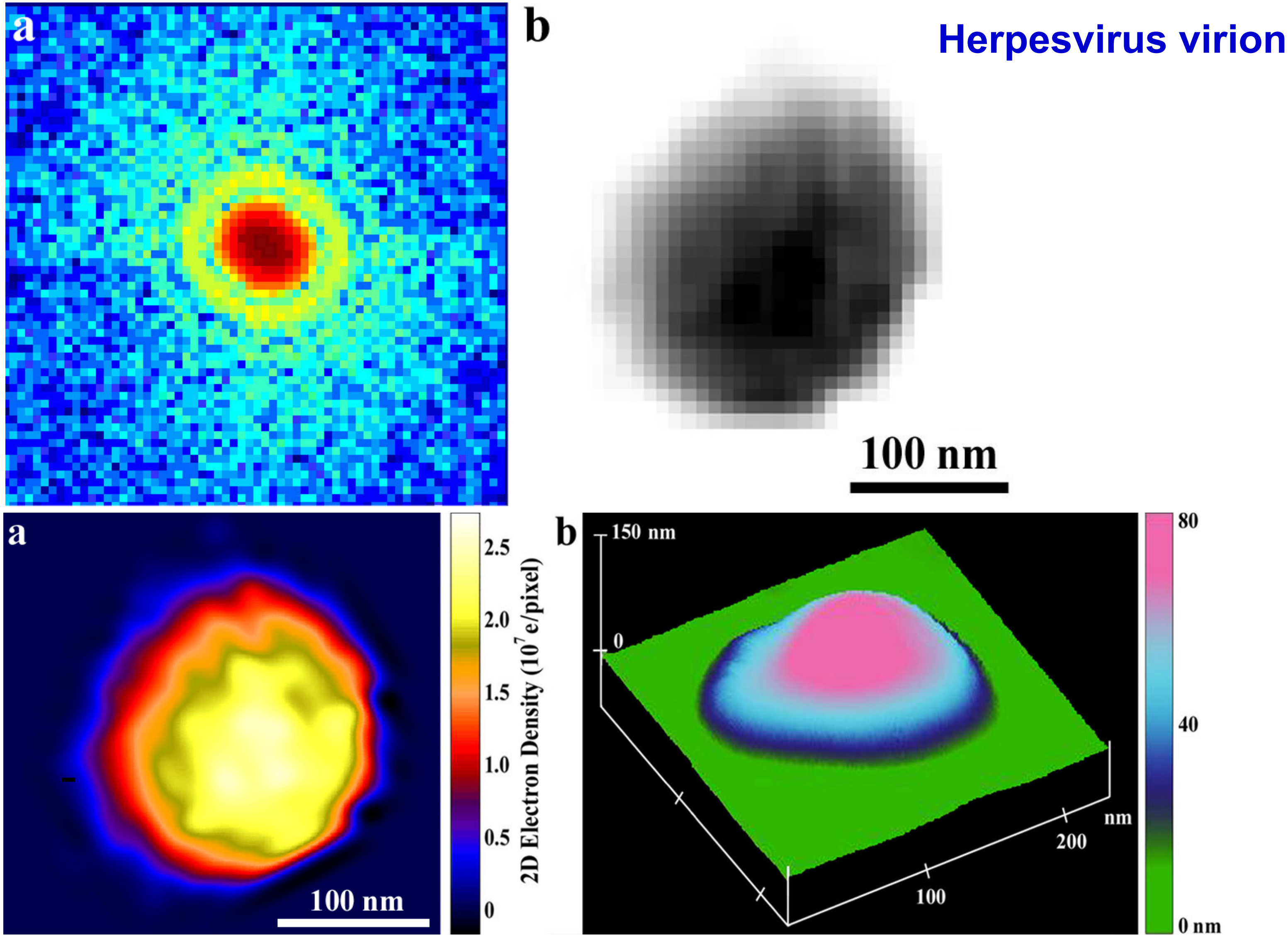
Radial expansion starts after 40ps with a speed of ~700 m/s (r_0 = 72 nm).

This represents the first experimental observation of irreversible melting.

Future plans: Improve the spatial resolution to the nanometer scale and the temporal resolution to femtoseconds.

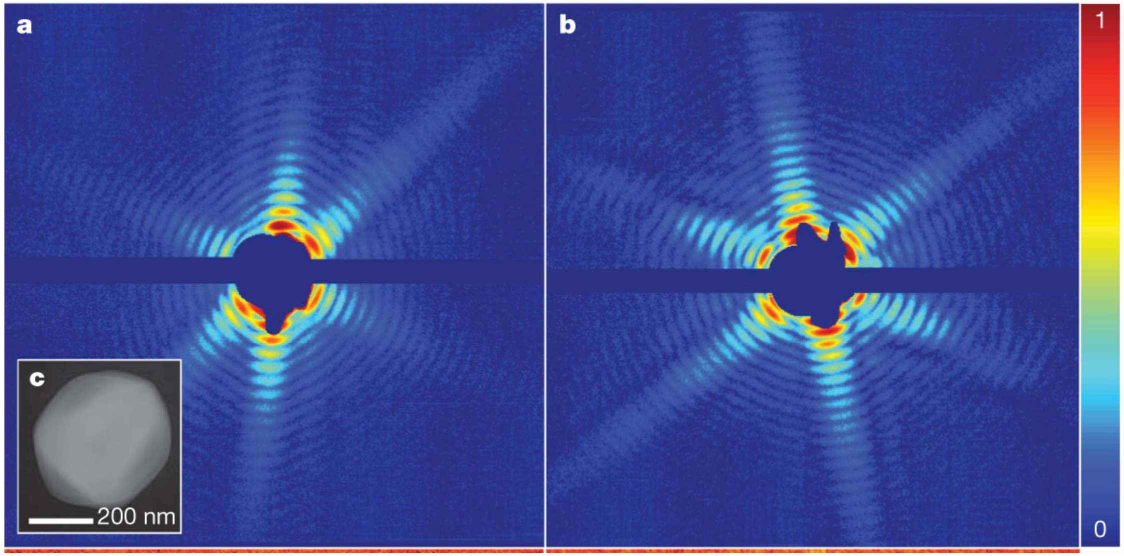
Ihm *et al.*, *Nat. Commun*. **10**, 2411 (2019).

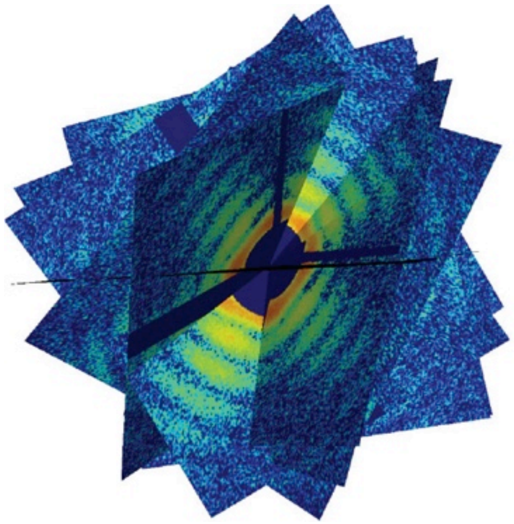
First Diffractive Imaging of a Single, Unstained Virion

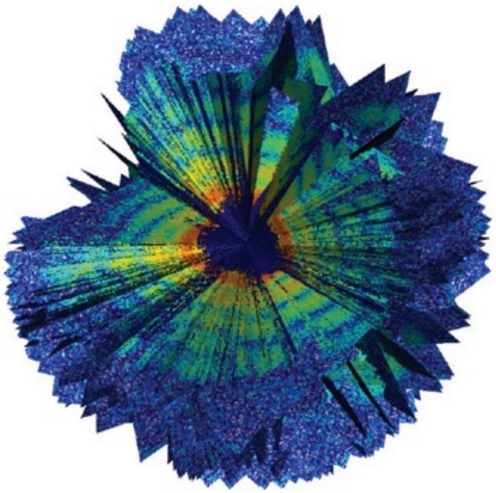


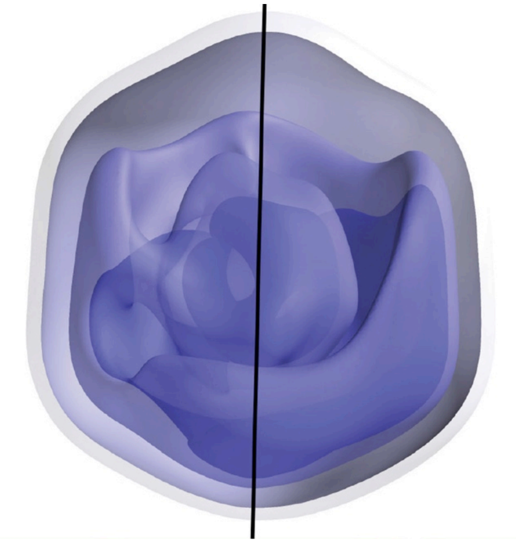
Song *et al.*, *PRL* **101**, 158101 (2008).

Diffractive Imaging of Single Mimiviruses Using LCLS



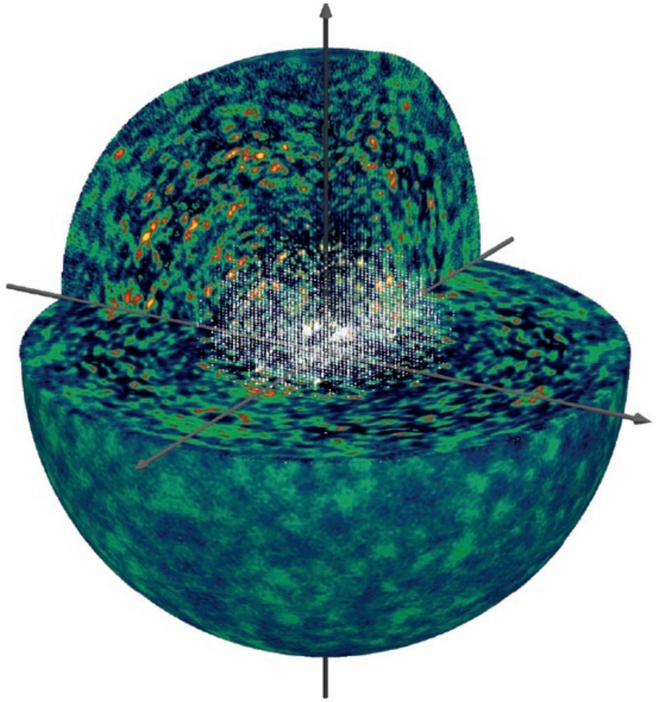


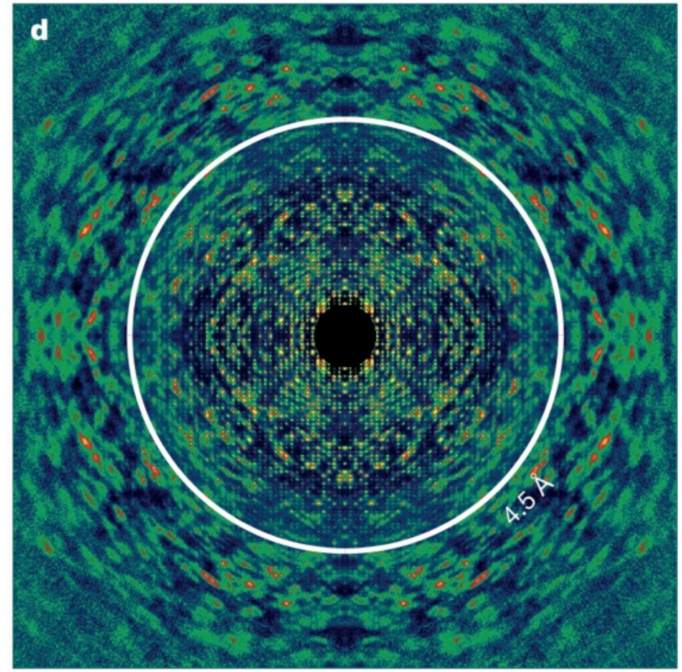




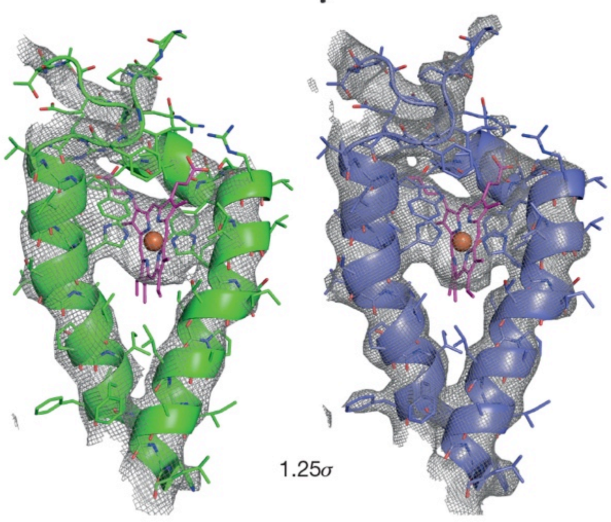
Seibert *et al*. *Nature* **470**, 78 (2011).
Ekeberg *et al*., *PRL* **114**, 098102 (2015).

Macromolecular Diffractive Imaging with the XFEL





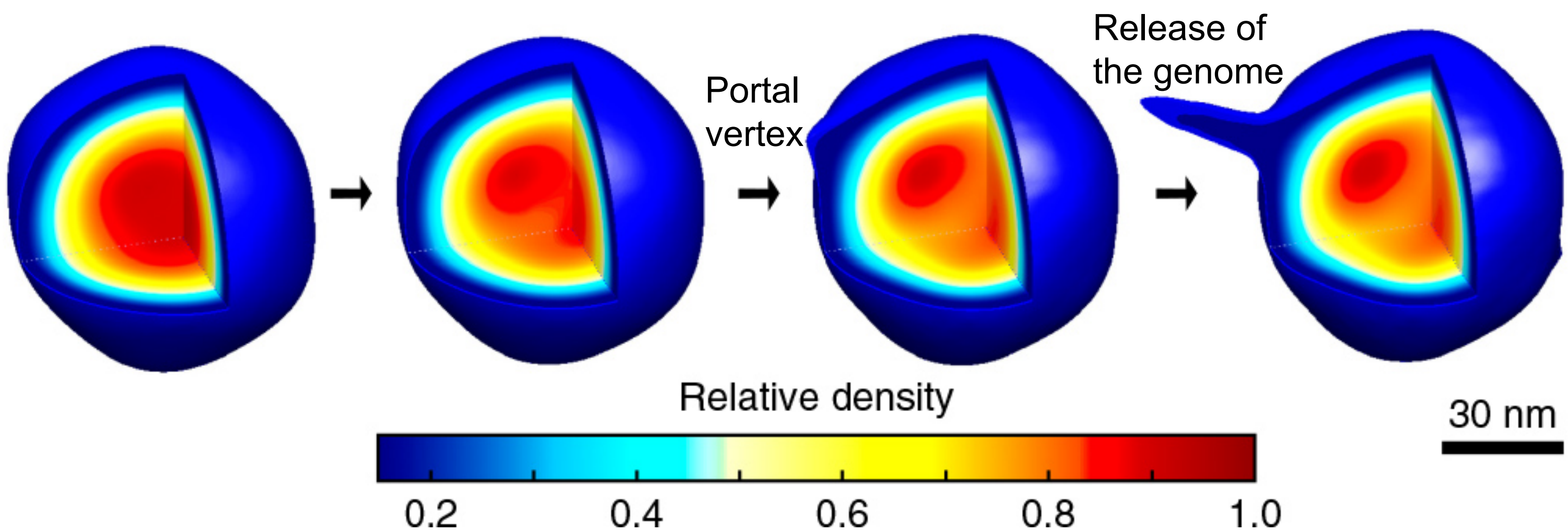
Continuous molecular diffraction pattern from imperfect crystals of photosystem II



Electron density maps of the haem group of PsbE/F using the Bragg diffraction (in green) and the Bragg and continuous diffraction (in blue).

Ayyer *et al*. *Nature* **530**, 202-206 (2016).

Capturing Conformational Changes in PR772 Viruses



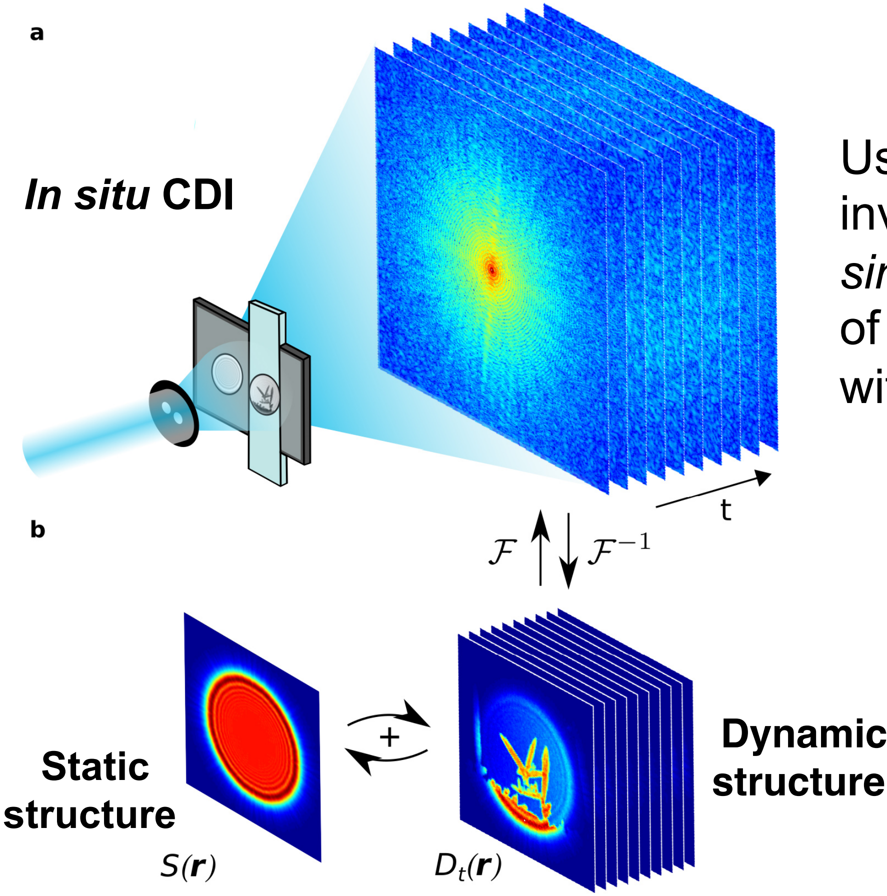
- 37,550 single-particle diffraction patterns
- 3D resolution: ~ 9 nm

Hosseinizadeh *et al*., *Nat. Methods* **14**, 877–881 (2017)

- **XFELs with higher photon flux per pulse**
- **Larger dynamic range detectors with single photon counting**
- **Dedicated sample preparation**
- **Advanced algorithms**
- **Complementary to cryo-EM**

In Situ CDI for Imaging Dynamic Systems

- **Ptychography uses partially overlapping regions in the space domain as a constraint.**
- ***In situ* CDI uses partially overlapping regions in the time domain as a constraint.**

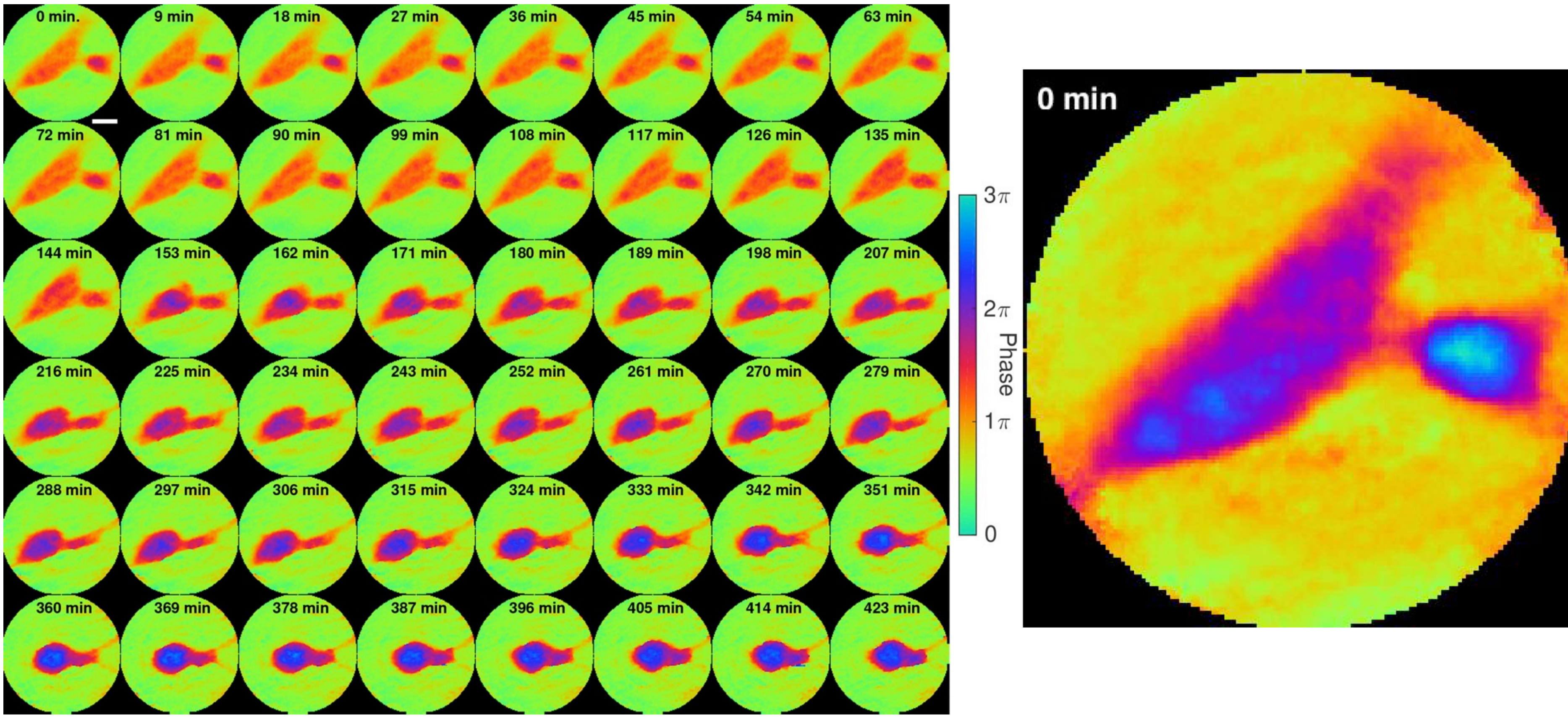


Using a static region as a powerful time-invariant constraint, *in situ* CDI can *simultaneously* reconstructs a time series of complex exit waves of dynamic systems with rapid convergence.

Lo, Gallagher-Jones, Rana, Zhao, Lodico, Xiao, Regan & Miao. *Nat. Commun.* **9**, 1826 (2018).

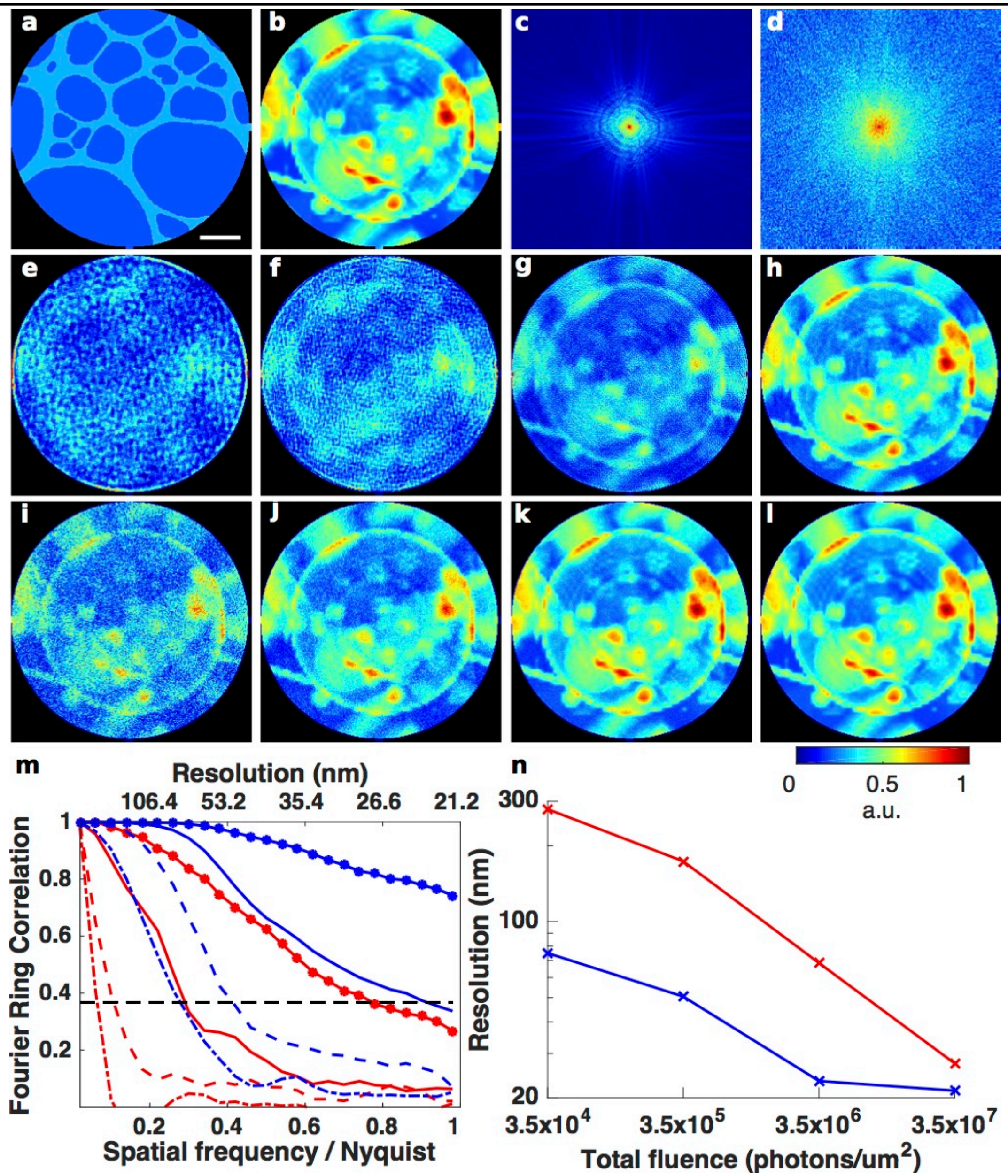
Proof-of-Principle Experiment on *In Situ* CDI of Live Cells

Phase images of the fusion of live cancer (glioblastoma) cells in culture medium



The experiment was conducted with an optical laser.

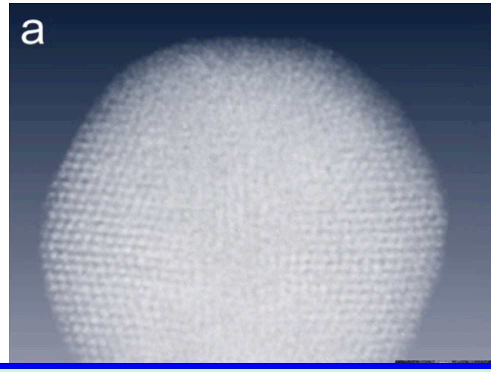
Numerical Simulations on Significant Dose Reduction Using *in situ* CDI

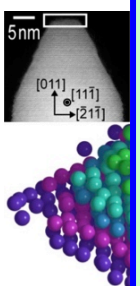


Lo, Gallagher-Jones, Rana, Zhao, Lodico, Xiao, Regan & Miao. *Nat. Commun.* **9**, 1826 (2018).

My Perspectives on Advanced Imaging with X-rays and Electrons

First experimental demonstration of AET (without assuming crystallinity)





Comparison between X-ray and electron imaging:

- **Electron imaging can achieve higher spatial resolution.**
- **Advanced X-ray imaging can reach high temporal resolution.**
- **X-rays have higher brilliance than electrons; seeded XFELs will be more impactful.**
- **Detectors, algorithms and big data are important for both imaging modalities.**

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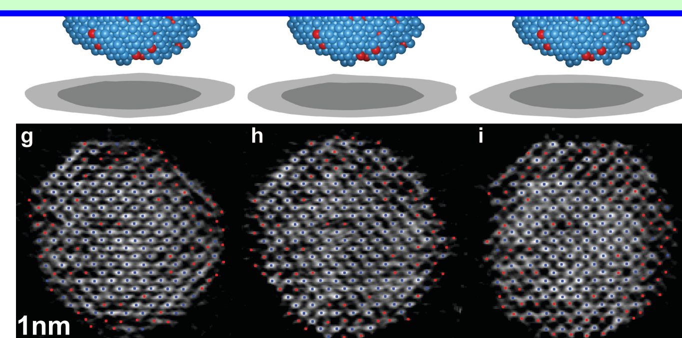
level

De
individual atoms with 19 pm precision



ng crystal
ion in 4D at
resolution;
Results differ from the classical nucleation theory.

Scott et al., *Nature* **483**, 444 (2012).
Chen et al., *Nature* **496**, 74 (2013).
Xu et al., *Nature Materials* **14**, 1099 (2015).
Miao et al., *Science* **353**, aaf2157 (2016).
Yang et al., *Nature* **542**, 75 (2017).
Zhou et al., *Nature* **570**, 500 (2019).

Summary

- Since the first experimental demonstration in 1999, CDI methods have been applied to image a wide range of samples in the physical and biological sciences.
- The combination of CDI and XFELs and HHG sources opens the door to probe the dynamics of materials with the nm spatial resolution and ps temporal resolution.
- We propose attoCDI for potential imaging of matter at the space-time limit, allowing the reconstruction of spectra, structures and illumination probes at different wavelengths.
- The ultimate goal of CDI is to image non-crystalline samples(such as single macromolecules) at near atomic resolution and on the femtosecond/attosecond time scales.
- With more brilliant X-ray sources such as XFELs, advanced synchrotron radiation, HHG and coherent electron sources, CDI in the next decade will be surely more exciting than the past one.

Acknowledgements

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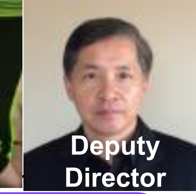
Software, codes and data are freely available: www.physics.ucla.edu/research/imaging

NSF STC on Real-Time Functional Imaging (STROBE)



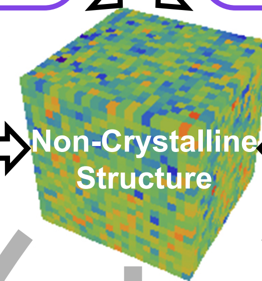
STROBE: Advance and integrate dynamic imaging techniques using electron, X-ray and nano-probe microscopy to collectively tackle major scientific and technological challenges

Capturing and monitoring individual atoms in 3D

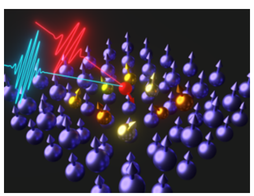
Routine 3D atomic resolution structure of biological complexes

Functional 3D imaging of energy, magnetic and spintronic materials

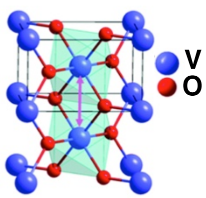
Imaging various forms of energy flow and fields across interfaces



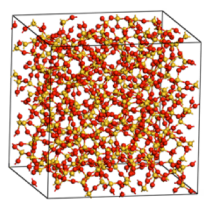
New windows into functional nanosystems



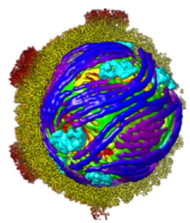
Energy materials



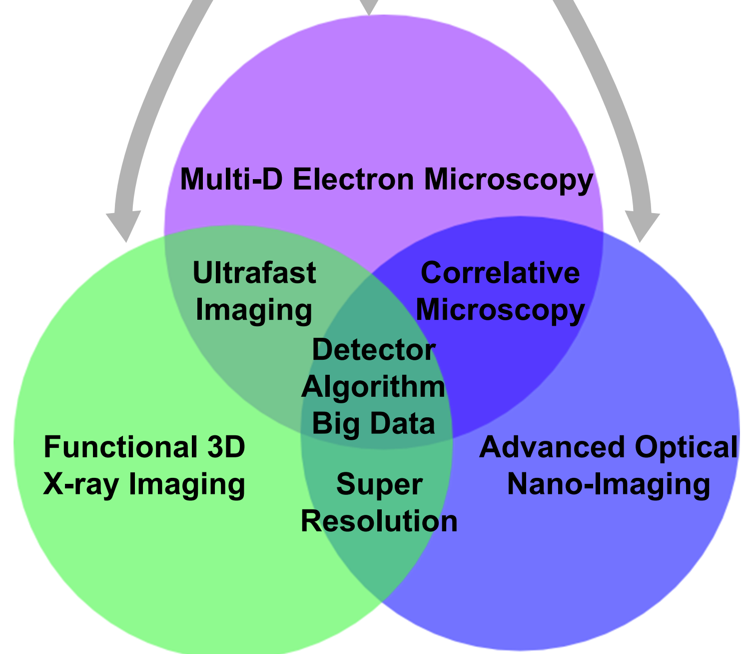
Quantum materials



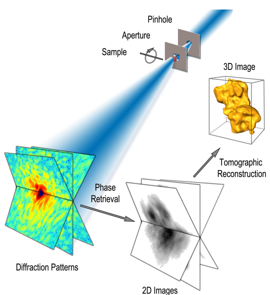
Disordered materials



Biological materials

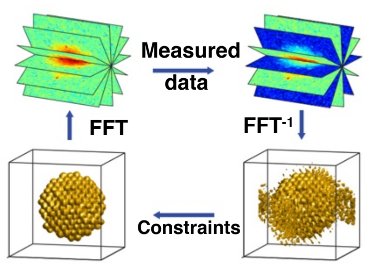


Advance and integrate dynamic imaging techniques



Techniques

Detectors, Big Data



Advanced Algorithms

University of Colorado Boulder | UCLA | Berkeley UNIVERSITY OF CALIFORNIA | FIU FLORIDA INTERNATIONAL UNIVERSITY | FORT LEWIS COLLEGE DURANGO, COLORADO | UC IRVINE