

# **NEED FOR SPEED**™

**High-throughput Materials  
Discovery via small-molecule  
serial femtosecond  
crystallography at LCLS**

Elyse Schriber, Associate Staff Scientist, LCLS

10/16/2025

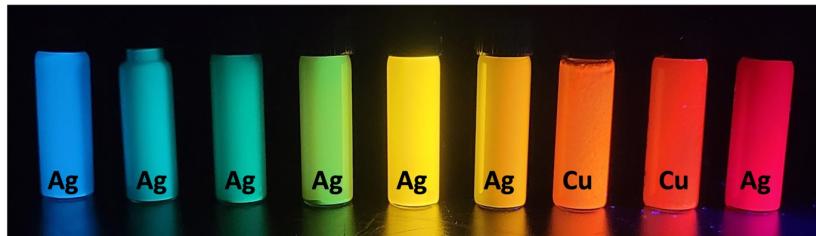
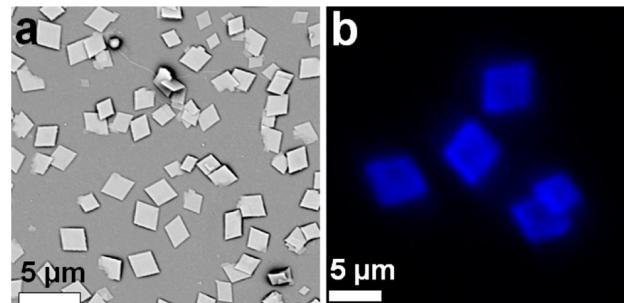


# Massive (or Micro) Bottleneck in Materials Discovery

SLAC

First MOChA synthesis reported in 2002,  
no reported high-quality structures until  
2020

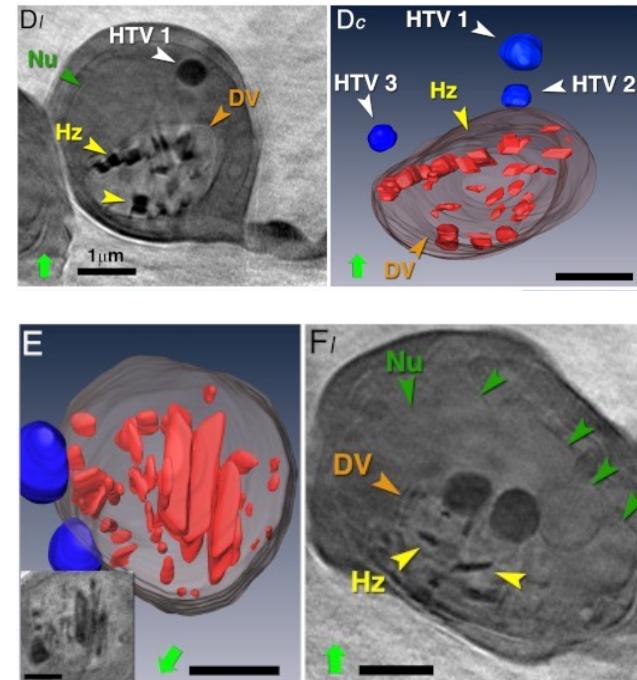
Metal-organic Chalcogenolates



A new field of hybrid materials with strong light-matter interactions that can be controlled by synthetic engineering via ligand/chalcogen exchange

30-year program with no structures of sufficient quality to explain observed properties.

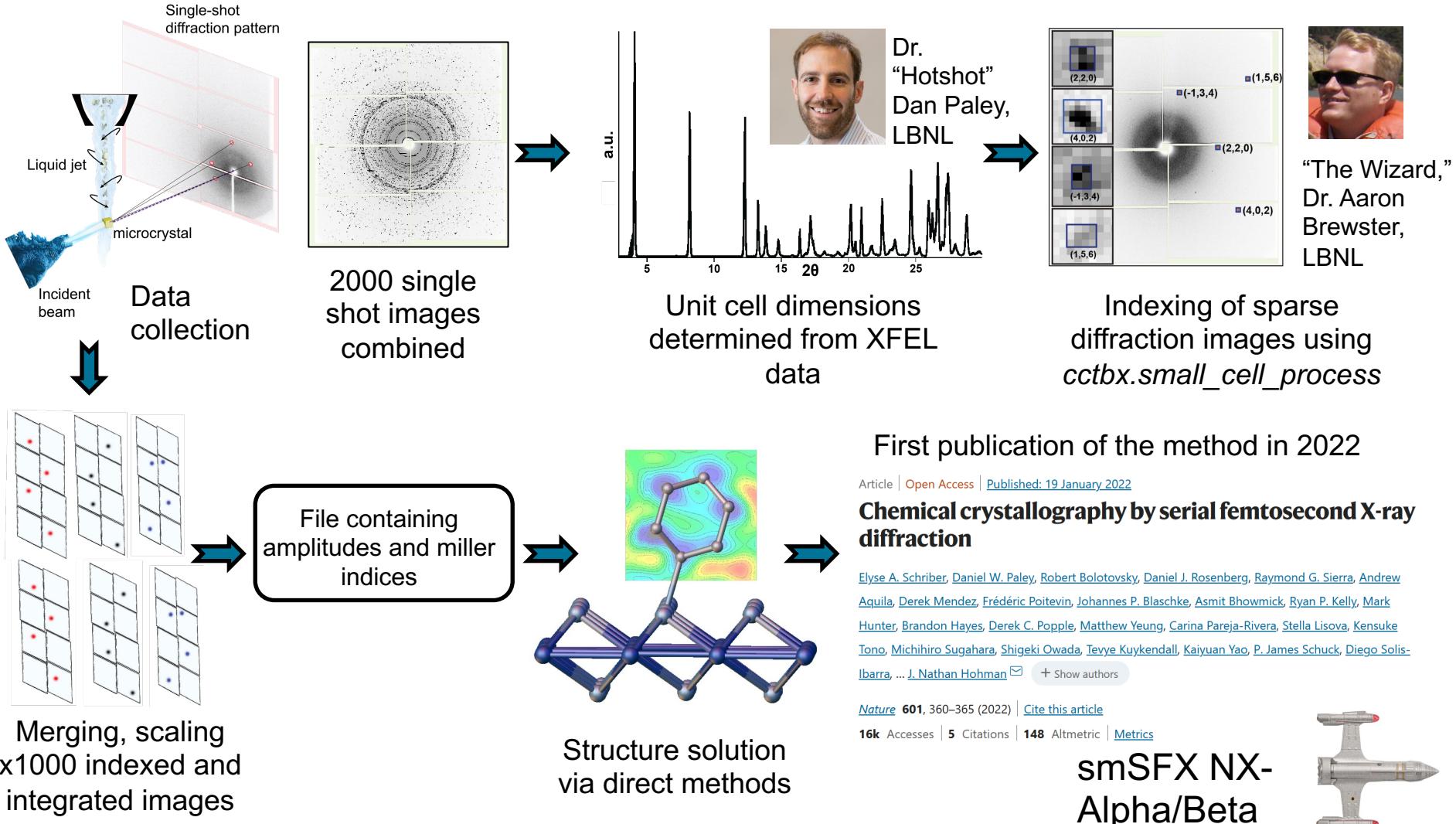
Hematin Anhydride ( $\beta$ -Hematin)



Synthetic analogue of Hemozoin, the microcrystalline Malaria pigment that is a drug target for antimalarials

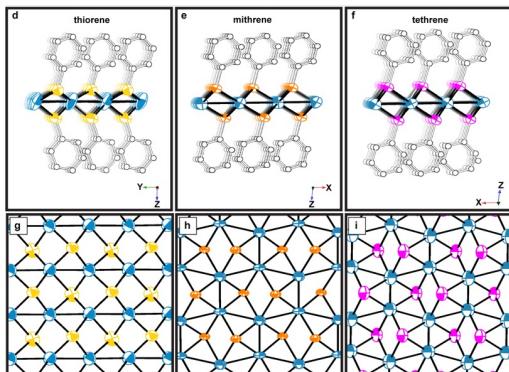
# Small-molecule Serial Femtosecond Crystallography: Warp 2.2

SLAC

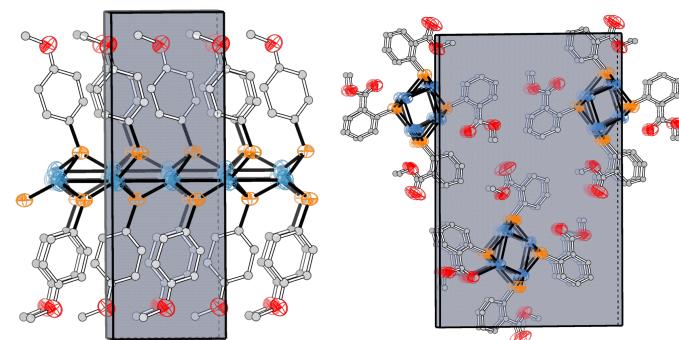


# Discoveries made during smSFX Warp 2.2

SLAC

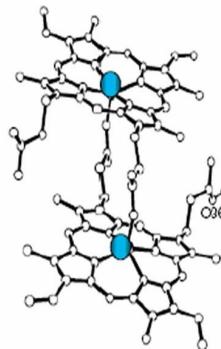


Optical divergence explained by inorganic sub-lattice geometry differences.

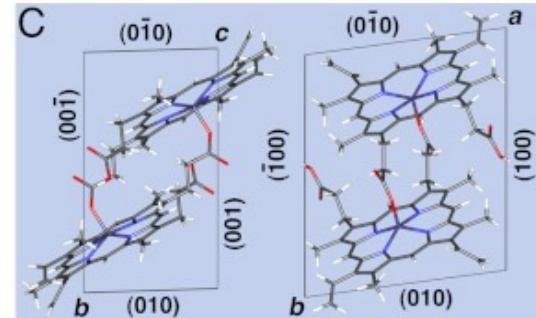


1D and 2D quantum confinement in a bulk material via ligand exchange

Discovered and characterized an exciting class of hybrid materials in the MOChas



Hematin Anhydride structure



Malaria Hemazoin structure

First high-resolution, high-quality single crystal structure of hematin anhydride, the synthetic analogue of hemazoin, that explains observed hydration and photo-active properties

## 55 Structures and counting since 2019!

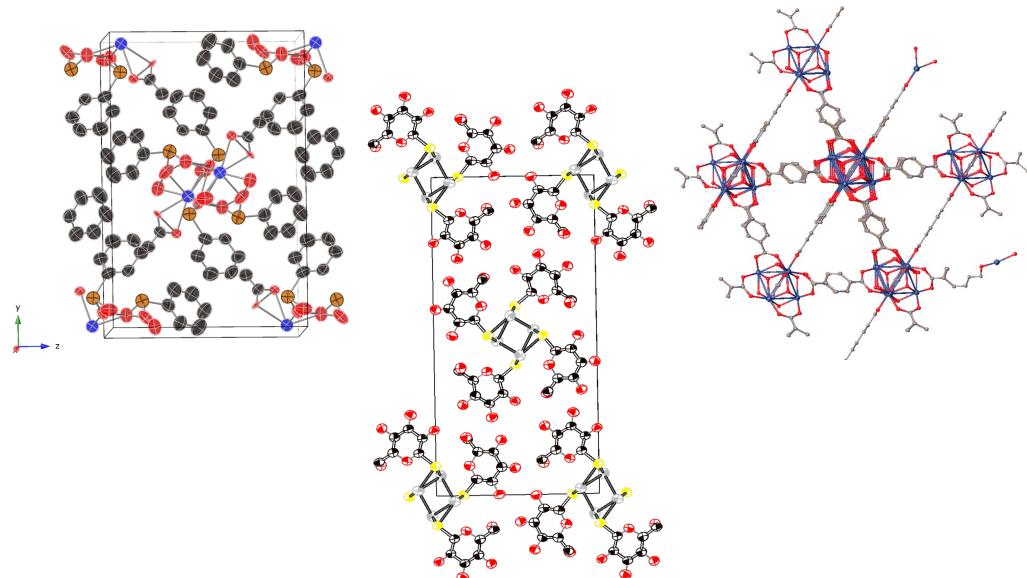
smSFX NX-Alpha/Beta



# Mail-In Chemical Crystallography Program at LCLS

SLAC

## The smSFX “Warp 2.2 Program”



### Additional Highlights

Determination of a single crystal structure of a new covalent organic framework that had eluded all other forms of structure determination (UC Berkeley)

Only made possible due to a strong, multi-year collaboration between UCONN, LCLS, and LBNL scientists.

### Mail-In smSFX I

- 48 h data collection
- 86 samples screened
- 18 different user groups
- 7 structures solved (8%)
- Fastest solved in 15 mins
- Rep Rate 120 Hz

### Mail-in smSFX II

- 24 h data collection
- 44 samples screened
- 14 different user groups
- 11 structures solved (25%)
- Rep Rate 30 Hz

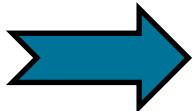
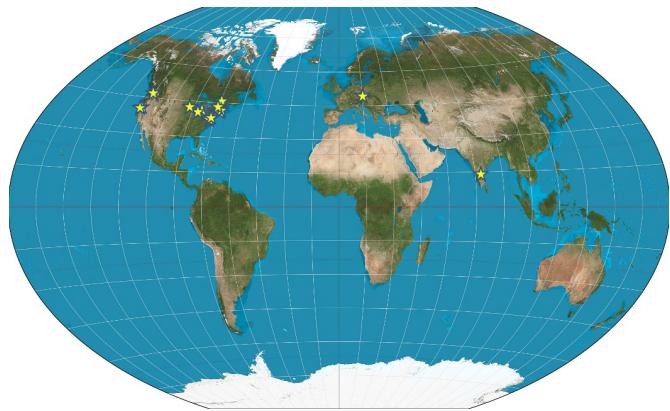
smSFX NX-  
Alpha/Beta



# smSFX During the LCLS-II HE Era “Warp 5 Program”

SLAC

Current mail-in smSFX outreach  
during the “Warp 2.2 Program”



- Starting to explore non-static smSFX capabilities at LCLS in Run 25

LCLS-II HE Era “Warp 5 Program”

- Complete datasets in 1-2 minutes
- Higher resolution datasets at 17-25 keV using large area detectors
- Advancing experimental methods for smSFX pump-probe diffuse scattering studies
- **Leveraging computational tools to drive efficiency and scientific discoveries using smSFX**



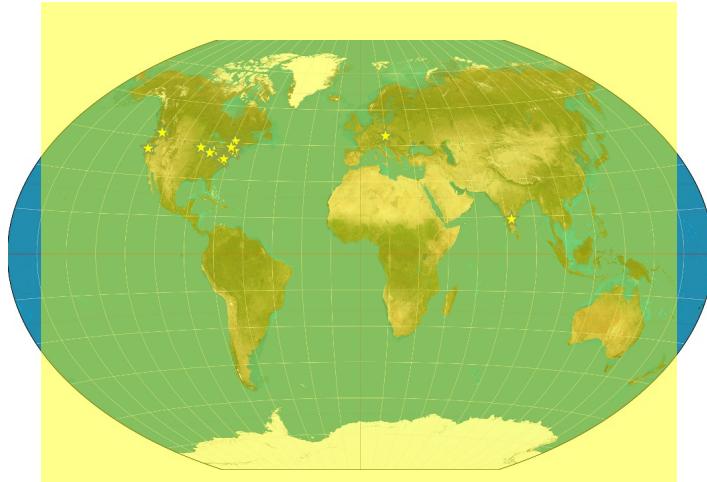
smSFX NX-  
Alpha/Beta

smSFX NX-01  
“Enterprise”



# smSFX During the LCLS-X Era “Warp 9.99 Program”

SLAC



Global Reach

- A dedicated endstation for smSFX.
- **The only XFEL mail-in smSFX program in the world, providing a regularly available global service.**
- Specialized endstation for pump-probe smSFX, chemical mixing experiments, and other non-static crystallography experiments.
- Large area detectors with a high QE at high photon energies (17-25 keV), **Super-resolution Crystallography?**
- Multimodal excitations, sample delivery, and sample environments



smSFX Galaxy-class NCC-1701 “Enterprise”