



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

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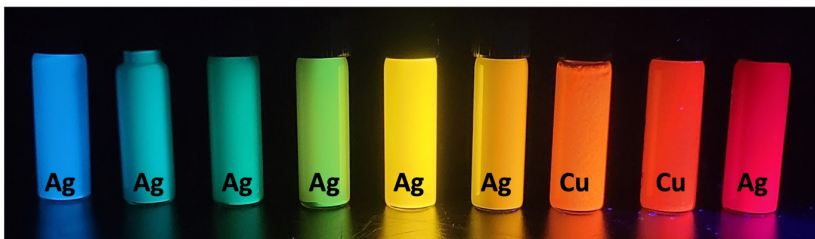
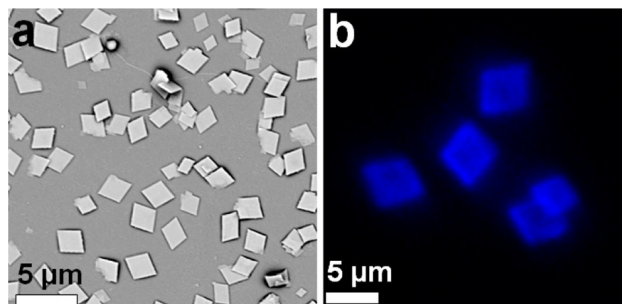


Massive (or Micro) Bottleneck in Materials Discovery

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

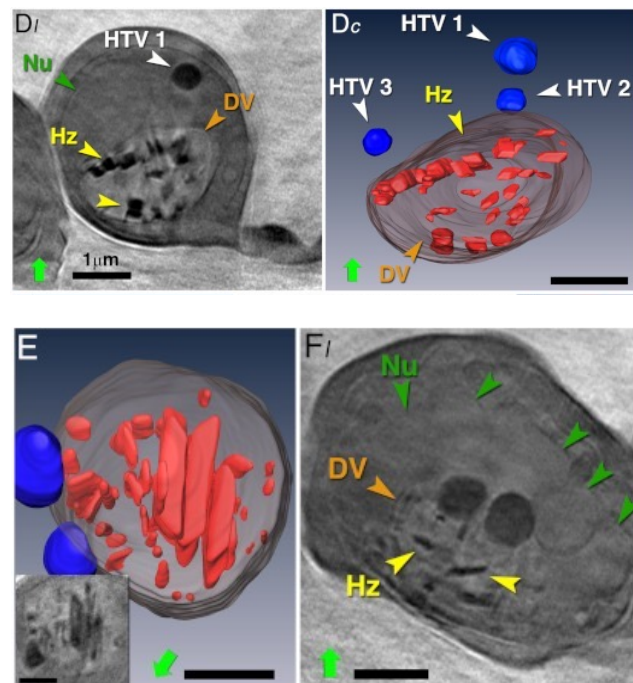
Metal-organic Chalcogenolates



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.

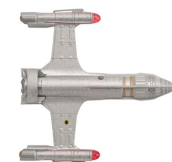
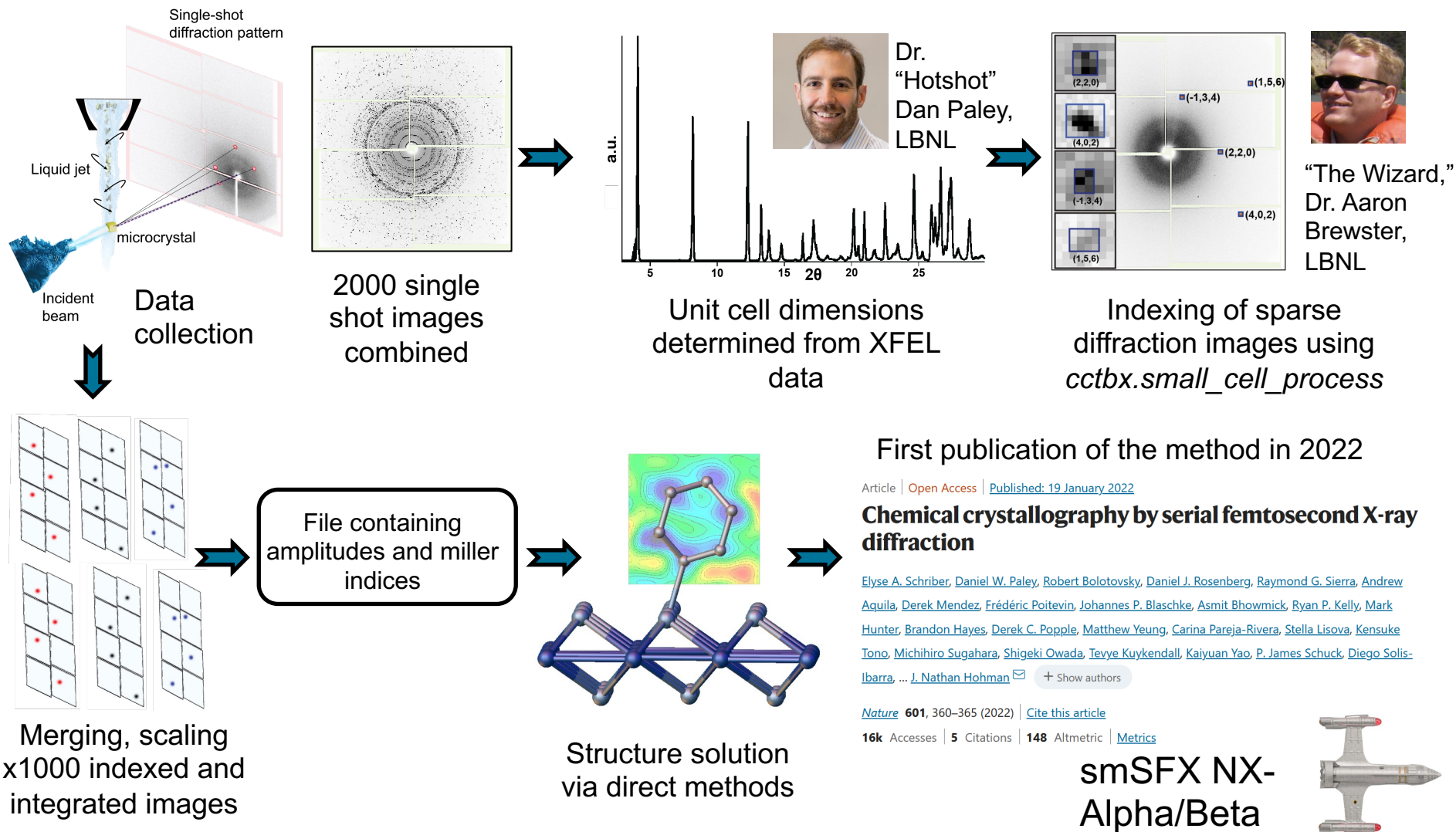
Hematin Anhydride (β -Hematin)



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

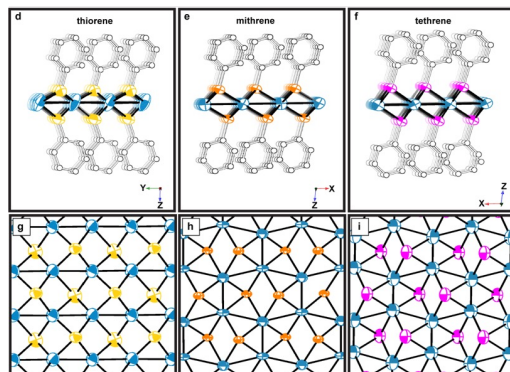
Small-molecule Serial Femtosecond Crystallography: Warp 2.2

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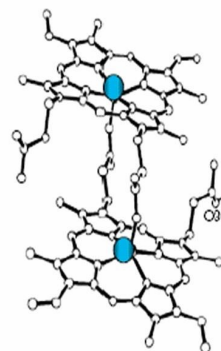


Discoveries made during smSFX Warp 2.2

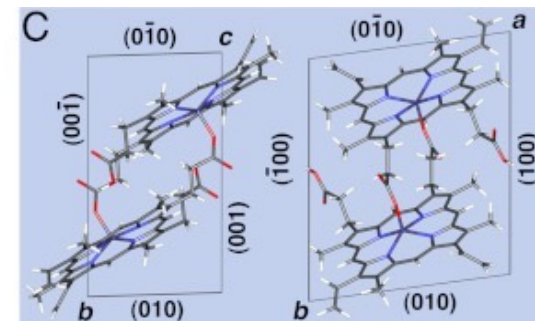
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Optical divergence explained by inorganic sublattice geometry differences.

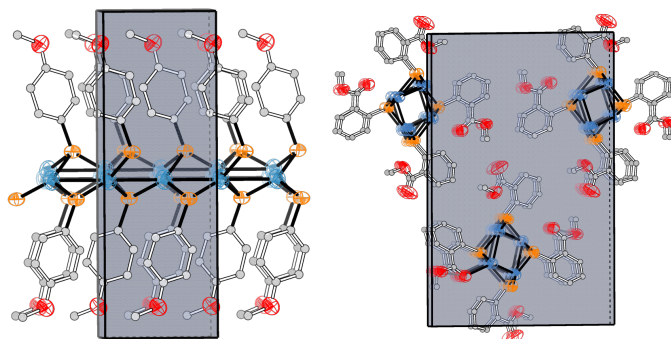


Hematin Anhydride structure



Malaria Hemazoin structure

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



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

55 Structures and counting since 2019!

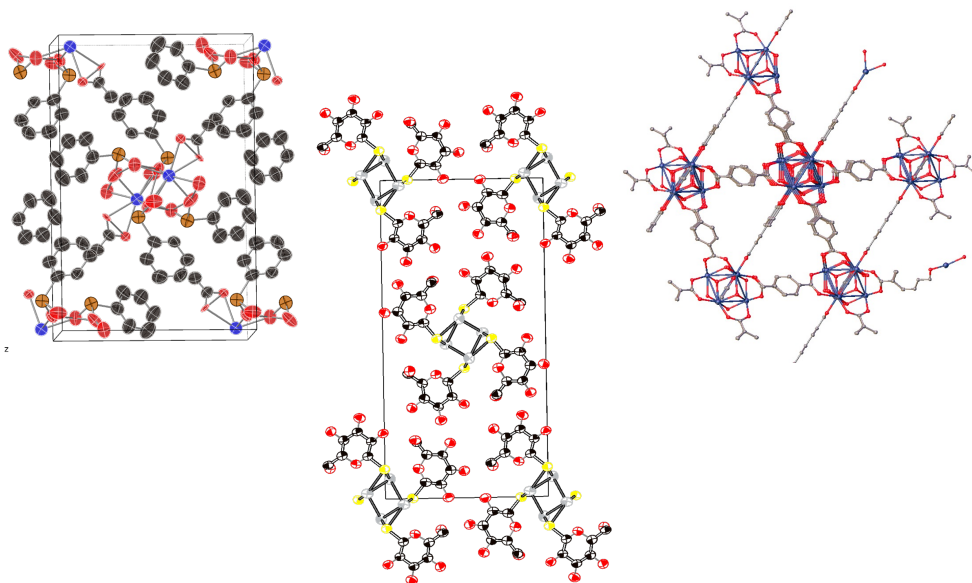
smSFX NX-Alpha/Beta



Mail-In Chemical Crystallography Program at LCLS

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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

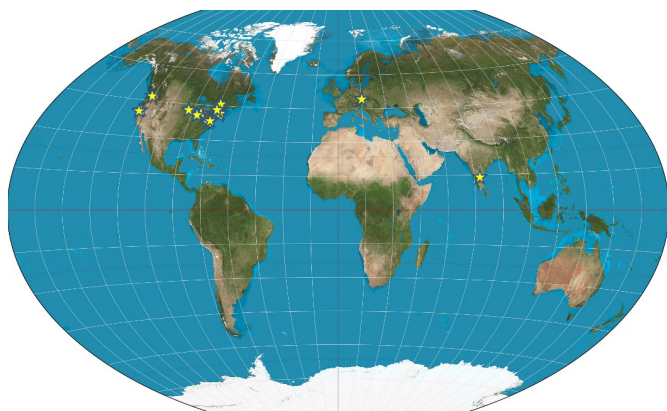
smSFX NX-
Alpha/Beta



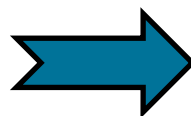
smSFX During the LCLS-II HE Era “Warp 5 Program”

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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

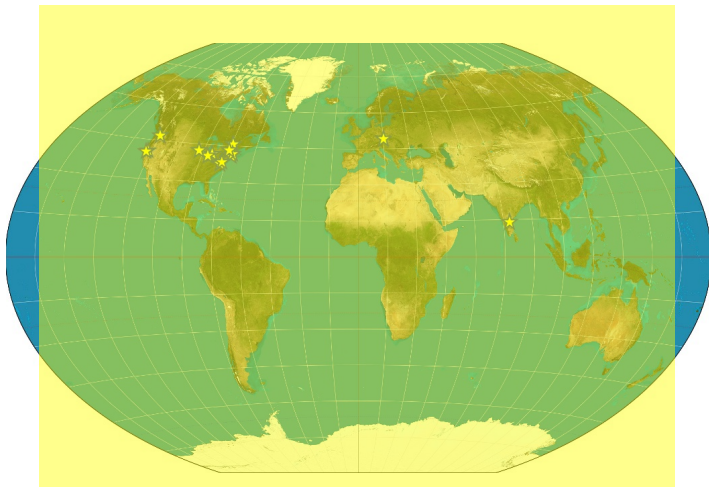


smSFX NX-01 “Enterprise”



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

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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”