Correlation Functions and Fluctuation X-ray Scattering and Imaging

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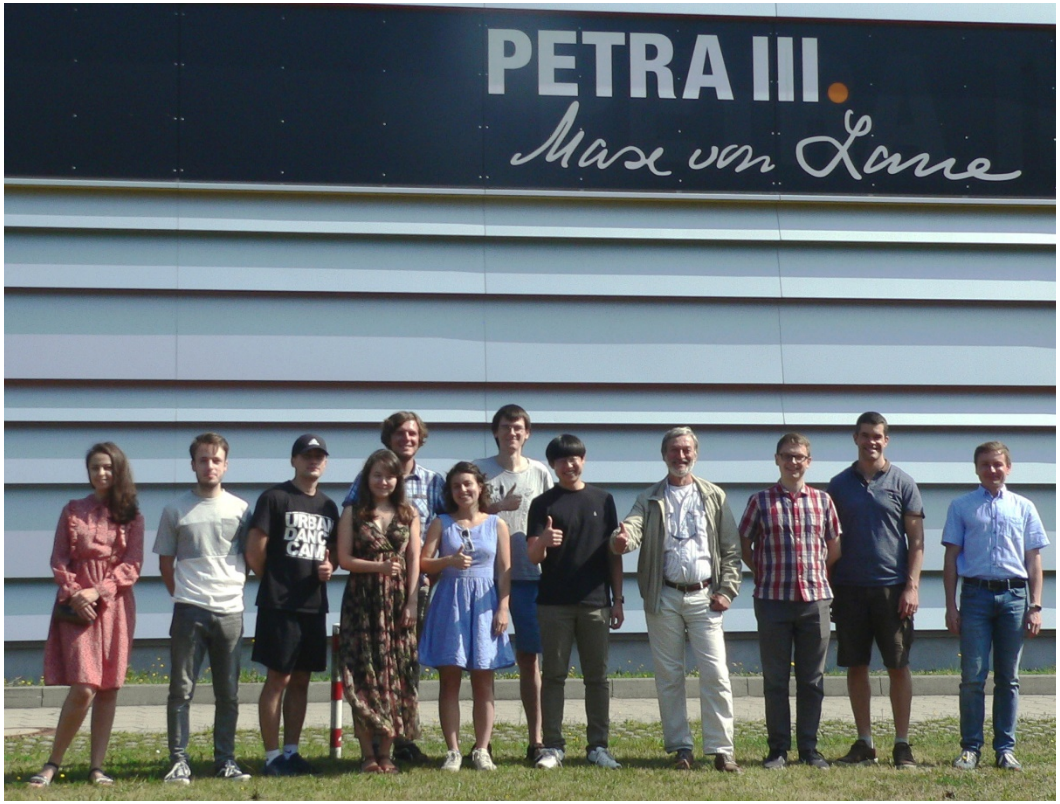
- A. Ignatenko
- R. Khubbutdinov
- S. Zolotarev (visitor)
- D. Egorov (summer student)
- S. Dubinina (summer student)



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Acknowledgments for this work

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- *F. Schreiber (University of Tubingen)*
- *M. Nielsen (DTU)*
- *and many others…*

Cross-correlation functions in signal processing

Cross-correlation functions

If we have two real random processes $x_1(t)$ and $x_2(t)$ then cross-correlation function is defined as

$$\Gamma(t_1, t_2) = \langle x(t_1) x(t_2) \rangle$$

Here averaging <…> is performed over different realizations of the random process

Normalized correlation function

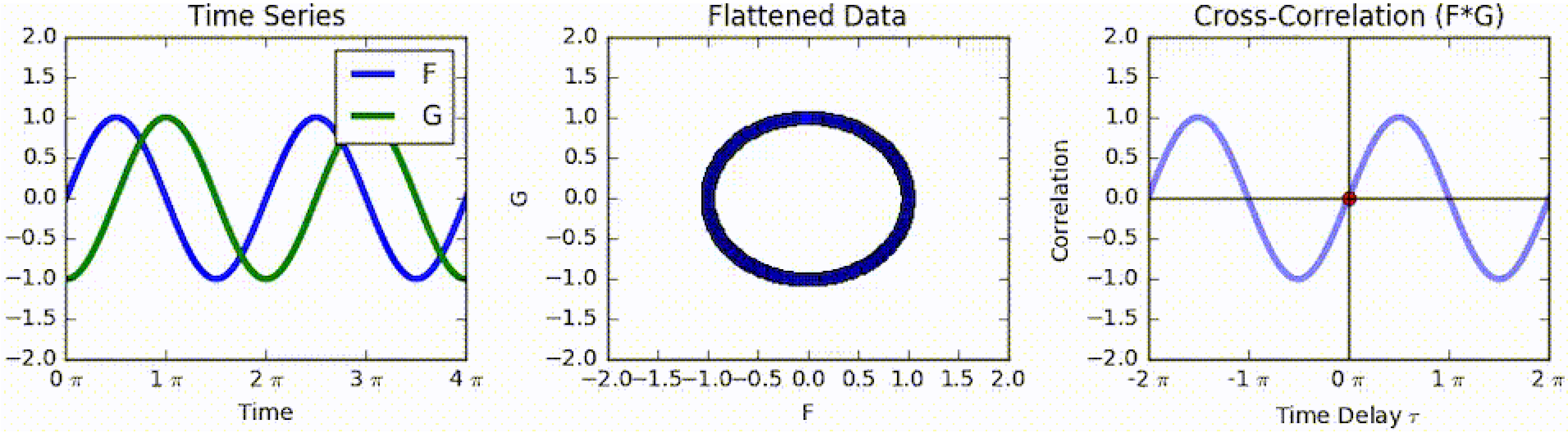
$$\gamma(t_1, t_2) = \frac{\Gamma(t_1, t_2)}{\sqrt{\Gamma(t_1, t_1)}\sqrt{\Gamma(t_2, t_2)}}$$

From Schwarz inequality

$$0 \le |\gamma(t_1, t_2)| \le 1$$

- When $|\gamma(t_1,t_2)|=0$ two processes $x_1(t)$ and $x_2(t)$ are not correlated
- When $|\gamma(t_1,t_2)|=1$ two processes $x_1(t)$ and $x_2(t)$ are completely correlated

Cross-correlation functions

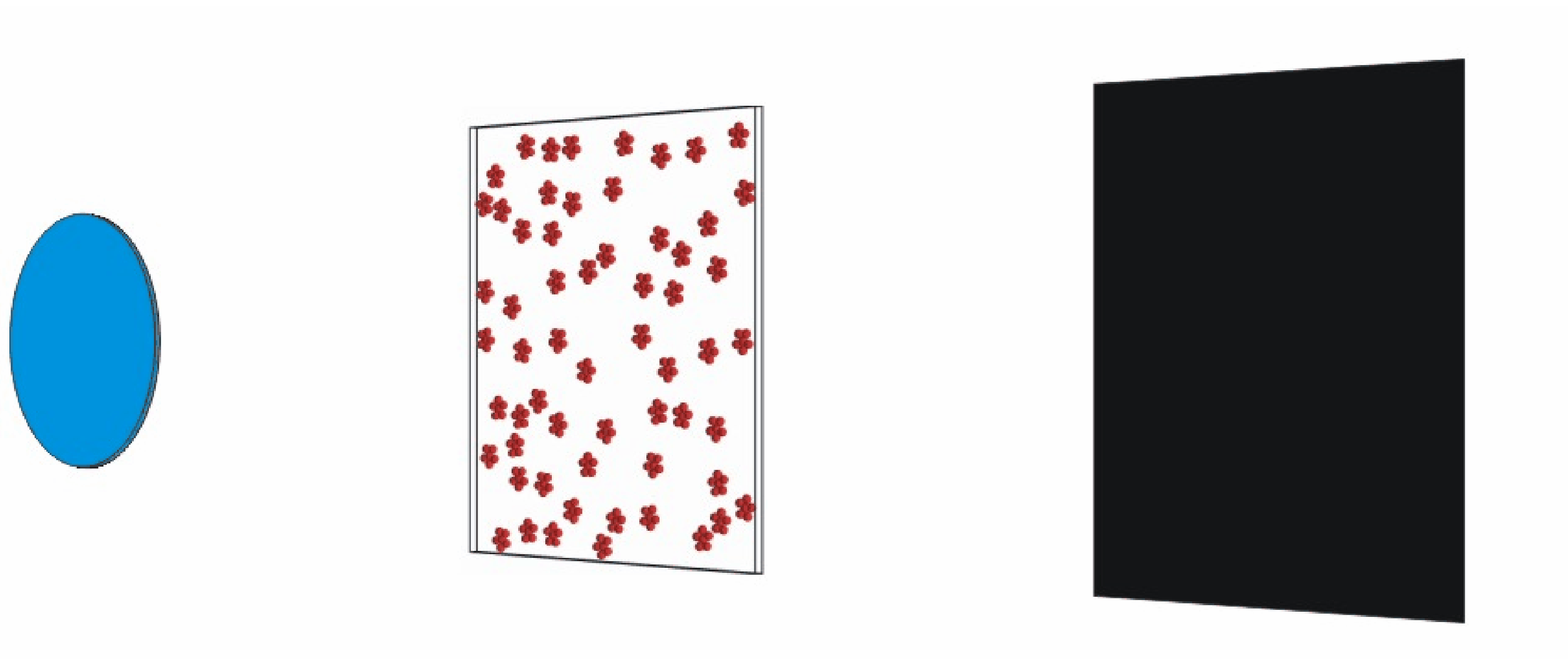


Cross-correlation of two functions F(t) and G(t):

$$F * G(\tau) = \int_{-\infty}^{\infty} F(t)G(t+\tau)dt$$

https://en.wikipedia.org/

Fluctuation X-ray Scattering



How to treat measured ensemble of diffraction patterns?

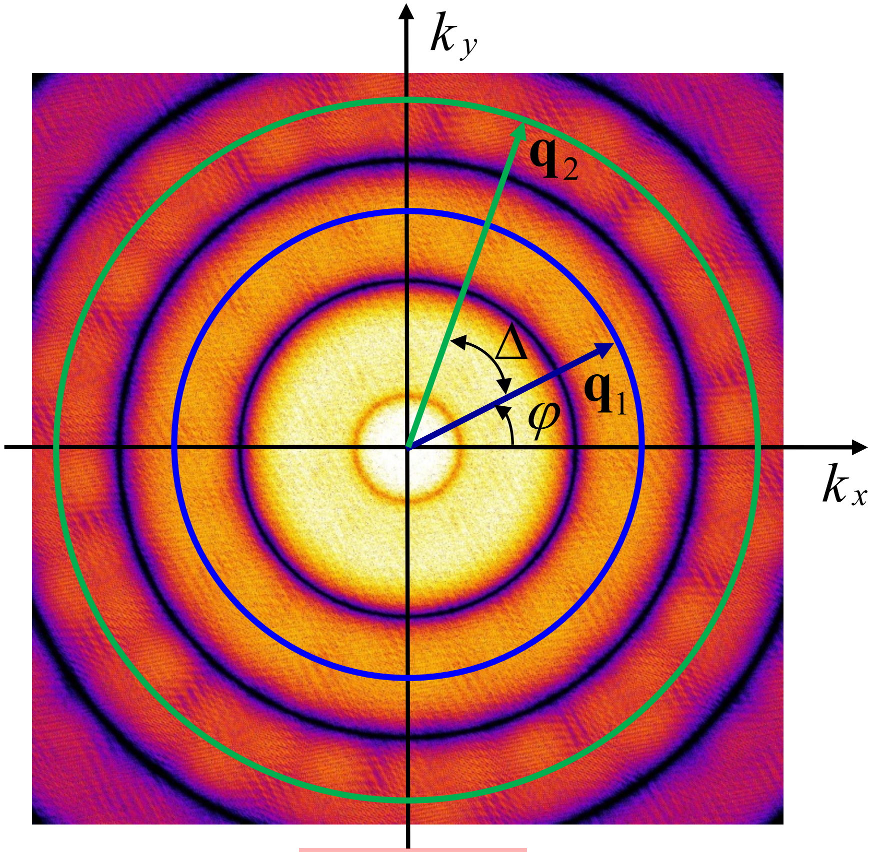
Single Particle Imaging (SPI) experiments

How to treat measured ensemble of diffraction patterns?

Definitions

Two-point angular cross-correlation function

Diffraction pattern
(N particles)



$|\mathbf{q}_1| \neq |\mathbf{q}_2|$

$$C(q_1, q_2, \Delta) = \langle I(q_1, \varphi) I(q_2, \varphi + \Delta) \rangle_\varphi$$

where $\langle \ldots \rangle_\varphi$ is an angular average

Fourier series of the CCF $C(q_1, q_2, \Delta)$:

$$C(q_1, q_2, \Delta) = \sum_{n=-\infty}^{\infty} C^n_{q_1,q_2} e^{in\Delta}$$

$$C^n_{q_1,q_2} = \frac{1}{2\pi} \int_0^{2\pi} C(q_1, q_2, \Delta) e^{-in\Delta} \, d\Delta$$

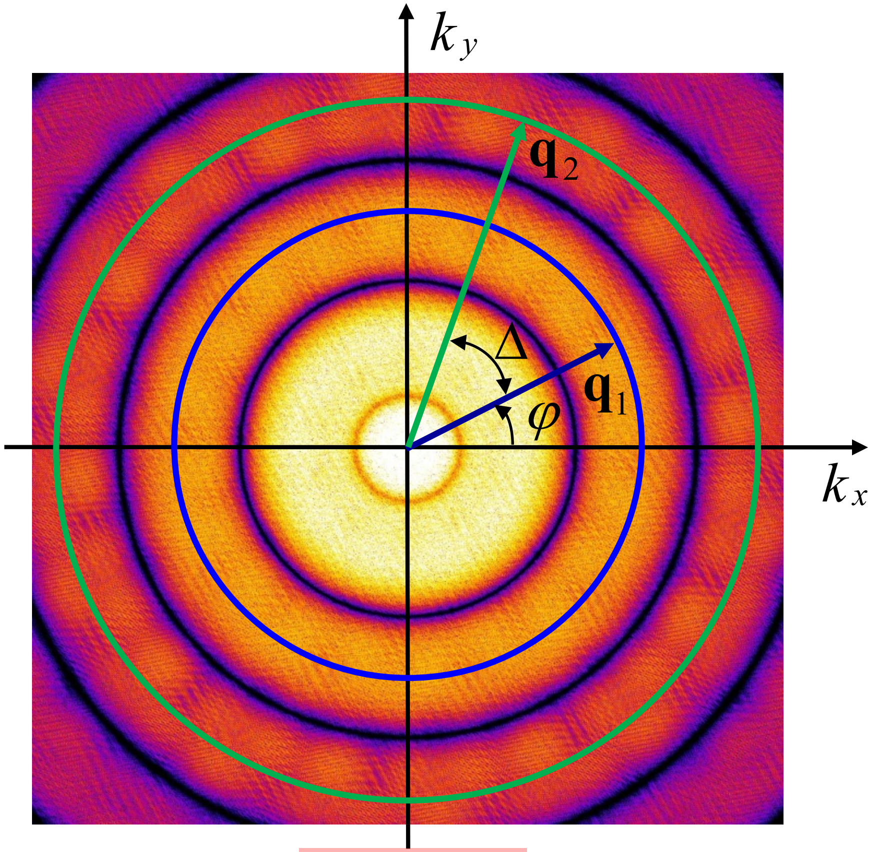
Applying convolution theorem:

$$C^n_{q_1,q_2} = I^{n^*}_{q_1} I^n_{q_2}$$

M. Altarelli, et al., Phys. Rev. B **82**, 104207 (2010)
R.P. Kurta, et al., Phys. Rev. B **85**, 184204 (2012)

Two-point angular cross-correlation function

Diffraction pattern
(N particles)



$|\mathbf{q}_1| \neq |\mathbf{q}_2|$

$$C(q_1, q_2, \Delta) = \langle I(q_1, \varphi) I(q_2, \varphi + \Delta) \rangle_{\varphi}$$

where $<\ldots>_{\varphi}$ is an angular average

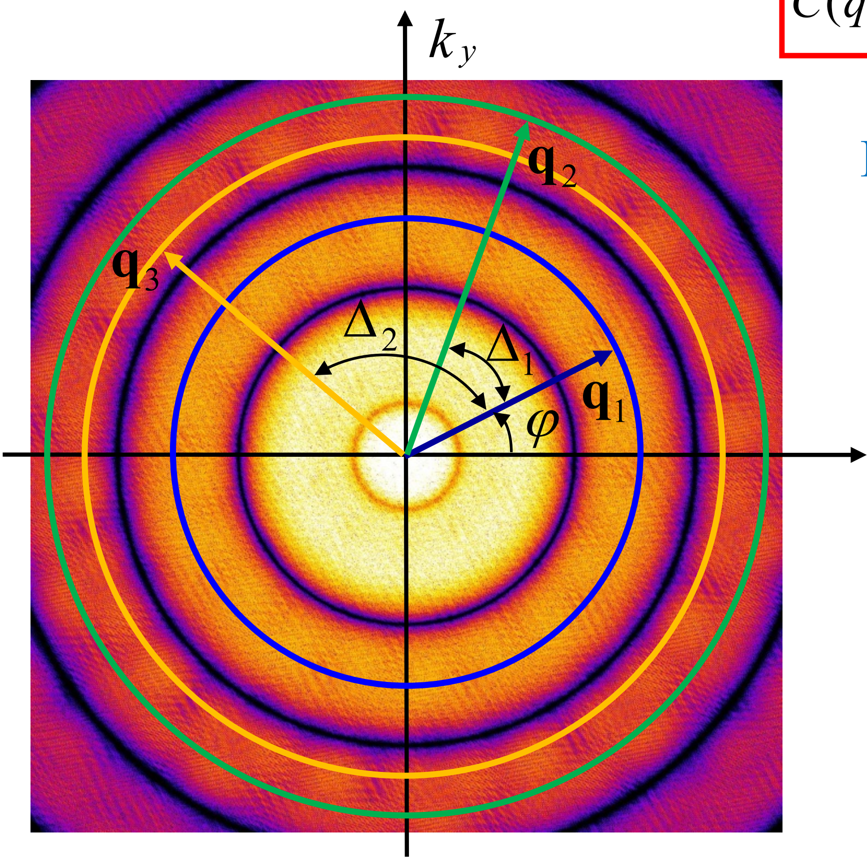
When we would have in diffraction pattern two peaks at momentum transfer vectors $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$, ACCF will have a peak at angle

$$\Delta = \widehat{\boldsymbol{q}_1 \boldsymbol{q}_2}$$

M. Altarelli, et al., Phys. Rev. B **82**, 104207 (2010)
R.P. Kurta, et al., Phys. Rev. B **85**, 184204 (2012)

Three-point angular cross-correlation function

Diffraction pattern
(N particles)



$$|\mathbf{q}_1| \neq |\mathbf{q}_2| \neq |\mathbf{q}_3|$$

Three-point CCF:

$$C(q_1, q_2, q_3, \Delta_1, \Delta_2) = \langle I(q_1, \varphi) I(q_2, \varphi + \Delta_1) I(q_3, \varphi + \Delta_2) \rangle_\varphi$$

Fourier series of the CCF $C(q_1, q_2, \Delta_1, \Delta_2)$:

$$C(q_1, q_2, q_3, \Delta_1, \Delta_2) = \sum_{n=-\infty}^{\infty} C_{q_1,q_2,q_3}^{n_1,n_2} e^{in_1\Delta_1} e^{in_2\Delta_2}$$

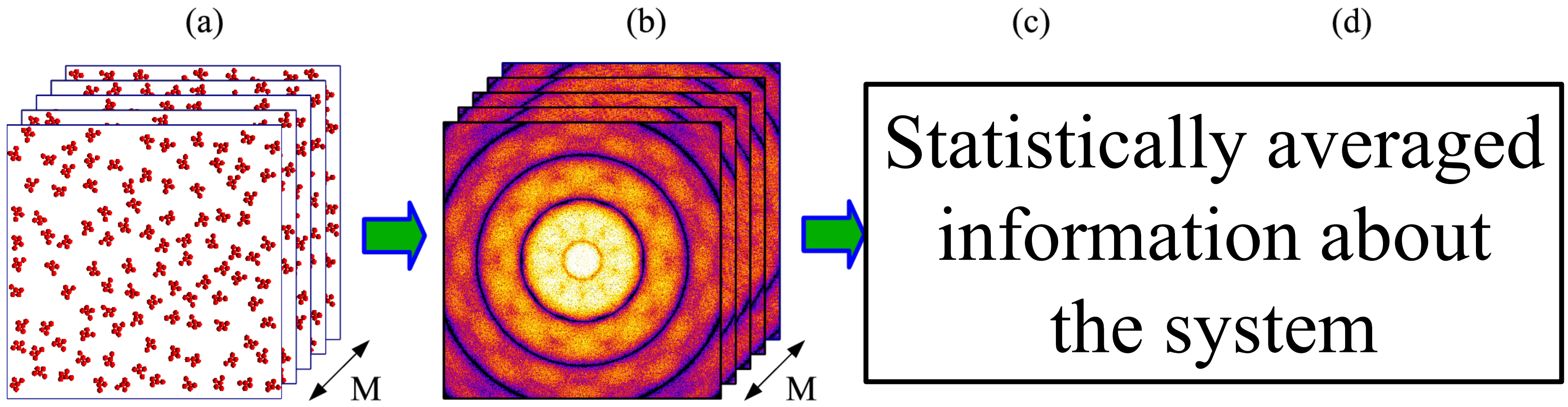
$$C_{q_1,q_2,q_3}^{n_1,n_2} \; C(q_1, q_2, q_3, \Delta_1, \Delta_2) =$$

$$\left[\frac{1}{2\pi}\right]^2 \iint_0^{2\pi} C(q_1, q_2, q_3, \Delta_1, \Delta_2)\, e^{in_1\Delta_1} e^{in_2\Delta_2} d\Delta_1 d\Delta_2$$

$$C_{q_1,q_2,q_3}^{n_1,n_2} = I_{q_1}^{(n_1+n_2)^*} I_{q_2}^{n_1} I_{q_3}^{n_2}$$

Z. Kam, *Macromolecules* **10**, 927 (1977)
Z. Kam, *J. Theor. Biol.* **82**, 1 (1980)

Analysis of ensemble averaged CCFs



(a) A large number *M* of realizations of a disordered system composed of *N* identical particles;

(b) Measured set of diffraction patterns;

(c) Statistically averaged information about the system

Analysis of ensemble averaged CCFs

CCF averaged over a sufficiently large number *M* of diffraction patterns

$$\left\langle C_q(\Delta)\right\rangle_M = 1/M\sum_{m=1}^{M} C_q^m(\Delta)$$

Fourier analysis

$$\left\langle C_q^n\right\rangle_M = 1/M\sum_{m=1}^{M}\left\{C_q^n\right\}_m$$

Long history of the use of angular cross-correlation functions in physics

Long history of the use of angular CCFs

Determination of Macromolecular Structure in Solution by Spatial Correlation of Scattering Fluctuations

Zvi Kam

Polymer Department, Weizmann Institute of Science, Rehovot, Israel.

Received April 11, 1977

Macromolecules, **10**, 927 (1977)

J. theor. Biol. (1980) **82**, 15–39

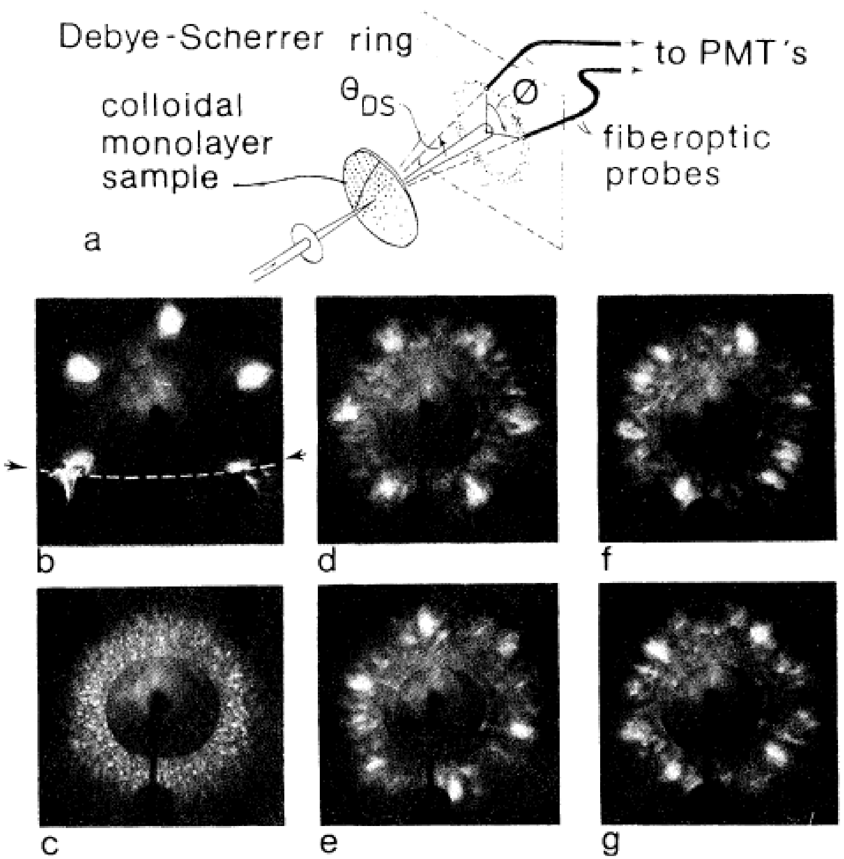
The Reconstruction of Structure from Electron Micrographs of Randomly Oriented Particles

ZVI KAM

Polymer Department The Weizmann Institute of Science Rehovot, Israel

Long history of the use of angular CCFs

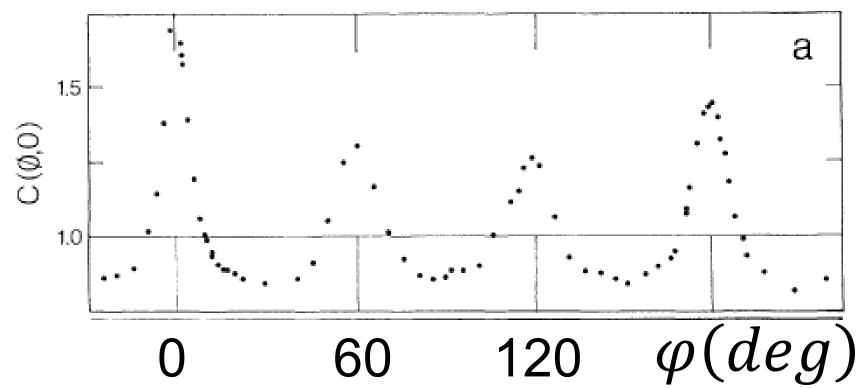
Scattering experiment on a charged polymer spheres in aqueous colloidal suspension



Photographs of typically observed scattered light distributions

Intensity cross-correlation function

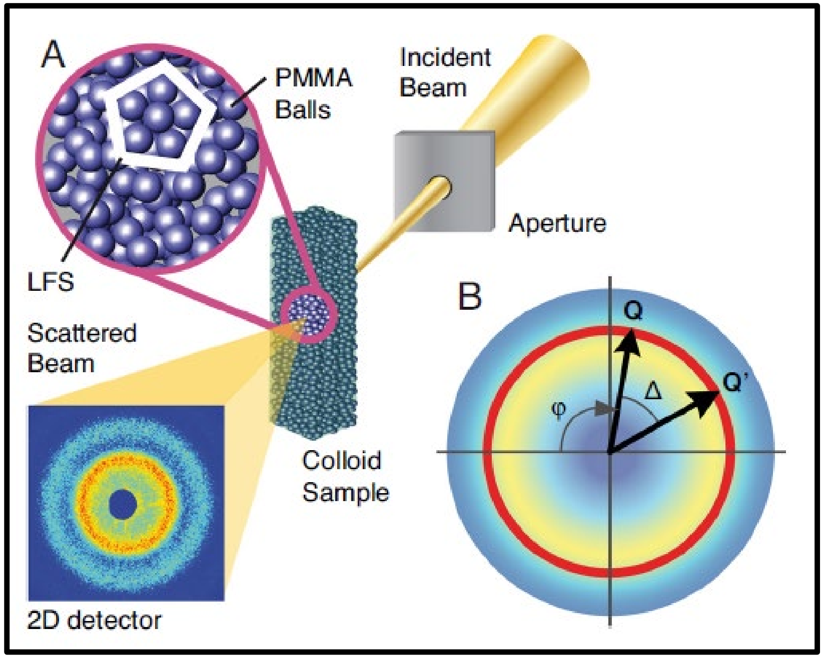
$$C(\varphi) = \frac{\langle I(q_1, \varphi = 0) I(q_2, \varphi) \rangle}{\langle I(q_1) \rangle \langle I(q_2) \rangle}$$

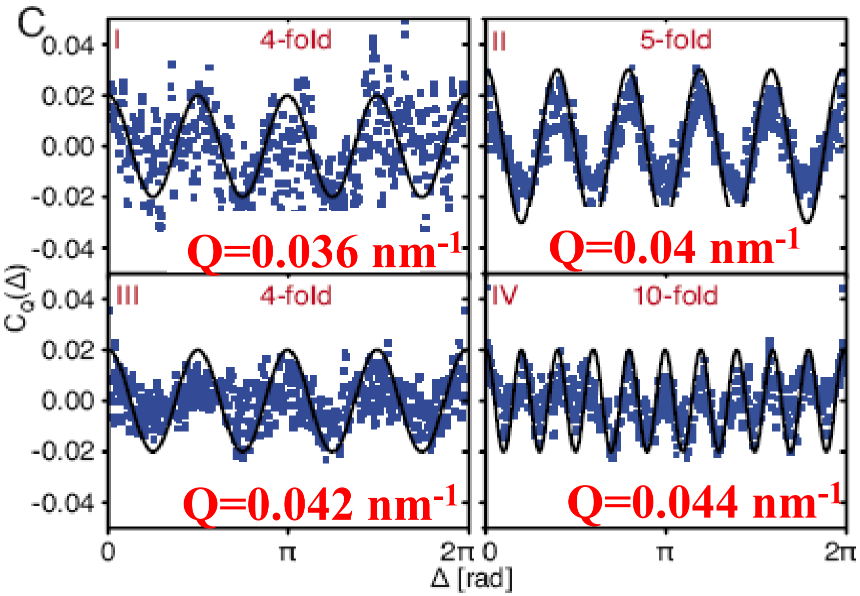


Measured intensity cross-correlation function in 2D liquid

Clark et al., PRL **50**, 1459 (1983)

Break down in 2009





Angular cross-correlation function

$$C_Q(\Delta) = \frac{\langle I(Q,\varphi)I(Q,\varphi+\Delta)\rangle_\varphi - \langle I(Q,\varphi)\rangle_\varphi^2}{\langle I(Q,\varphi)\rangle_\varphi^2}$$

Wochner P *et al.*, PNAS **106**, 11511 (2009)

Our work

First publications:

- M. Altarelli, R.P. Kurta, and I. A. Vartanyants, Phys. Rev. B **82** 104207 (2010).
- R.P. Kurta, M. Altarelli, E. Weckert and I. A. Vartanyants, Phys. Rev. B **85** 184204 (2012).
- R.P. Kurta, R. Dronyak, M. Altarelli, E. Weckert, and I.A. Vartanyants, New J. Phys. **15** 013059 (2013).

Reviews:

- R.P. Kurta, M. Altarelli, and I.A. Vartanyants, Adv. Cond. Matter Phys. 959835, (2013)
- R. Kurta, M. Altarelli, and I.A. Vartanyants, Adv. Chem. Phys., v. **161**, Eds. S. A. Rice&A. R. Dinner. (2016), pp. 1-39
- I. Zaluzhnyy, R. P. Kurta, M. Scheele, F. Schreiber, B. I. Ostrovskii, and I. A. Vartanyants, Materials, **12**, 3464 (2019).

Application to different systems:

- Hexatic phase of liquid crystals
- Mesocrystals formed from nanocrystals
- Dynamics of molecules in liquids

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X-ray cross-correlation analysis of free-standing liquid crystal films

R. Kurta *et al.*, Phys. Rev. E Brief Reports **88**, 044501 (2013)
I. Zaluzhnyy *et al.*, Phys. Rev. E **91**, 042506 (2015)
I. Zaluzhnyy *et al.*, Phys. Rev. E **94**, 030701(R) (2016)
I. Zaluzhnyy *et al.*, Soft Matter **13**, 3240 (2017)
I. Zaluzhnyy *et al.*, Mol. Cryst. Liq. Cryst., **647**, 169 (2017)
I. Zaluzhnyy *et al.*, Phys. Rev. E, **98**, 052703 (2018)

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Applications

Liquid crystal displays (LCDs)

Polymer dispersed liquid crystal devices (smart glasses)

Liquid crystal tunable filters (LCTFs)

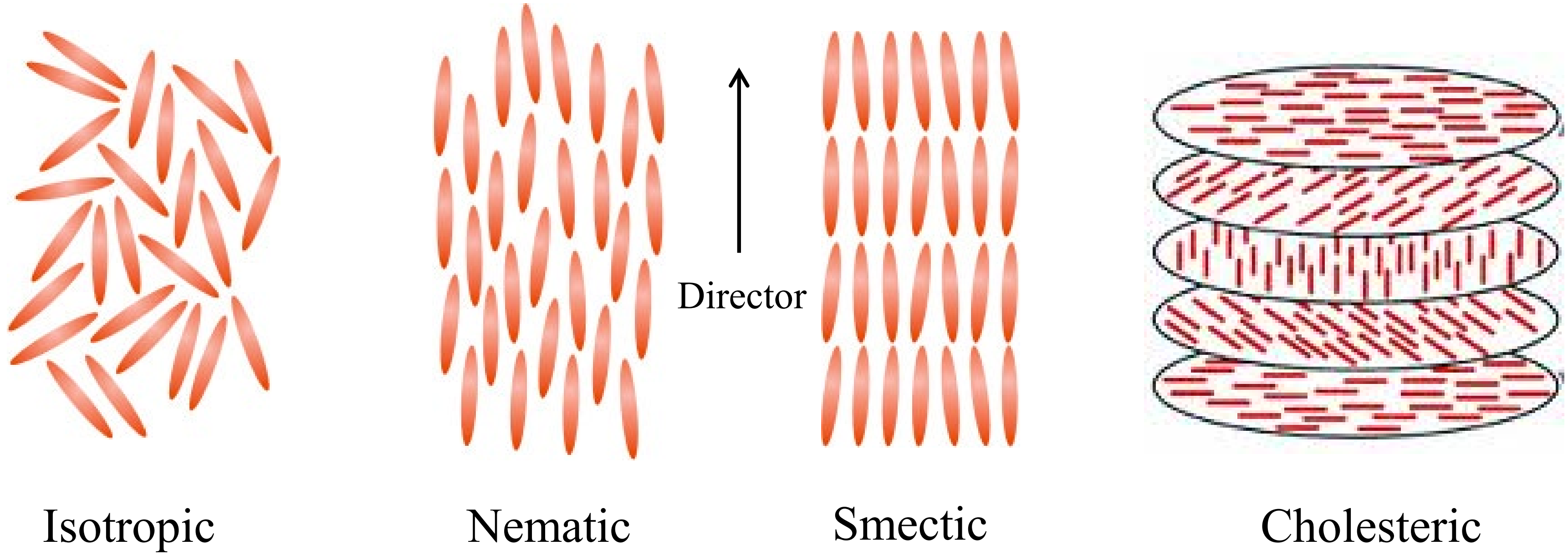
Soap

Liquid crystal thermometers

http://wikipedia.org

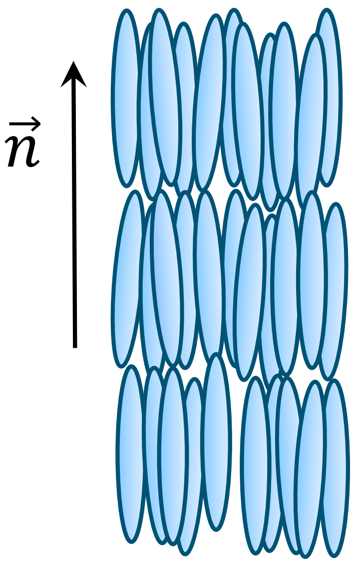
DESY

Liquid crystal phases

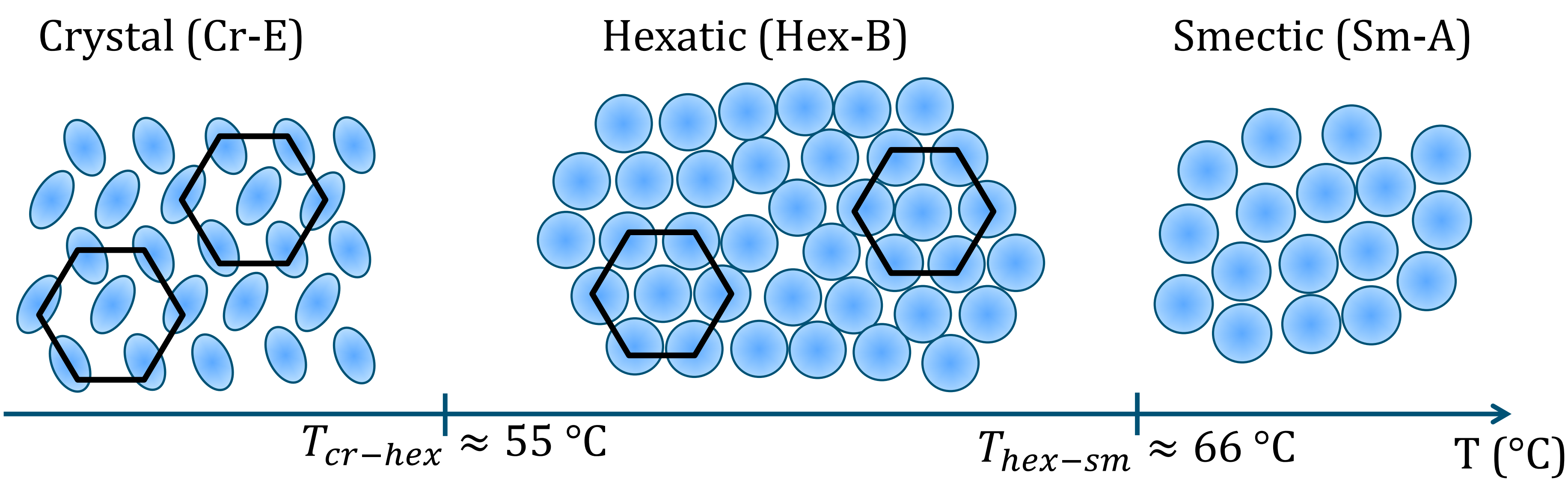


Molecular structure of a typical rod-shaped liquid crystal (LC) molecule

Smectic and hexatic phases in liquid crystals



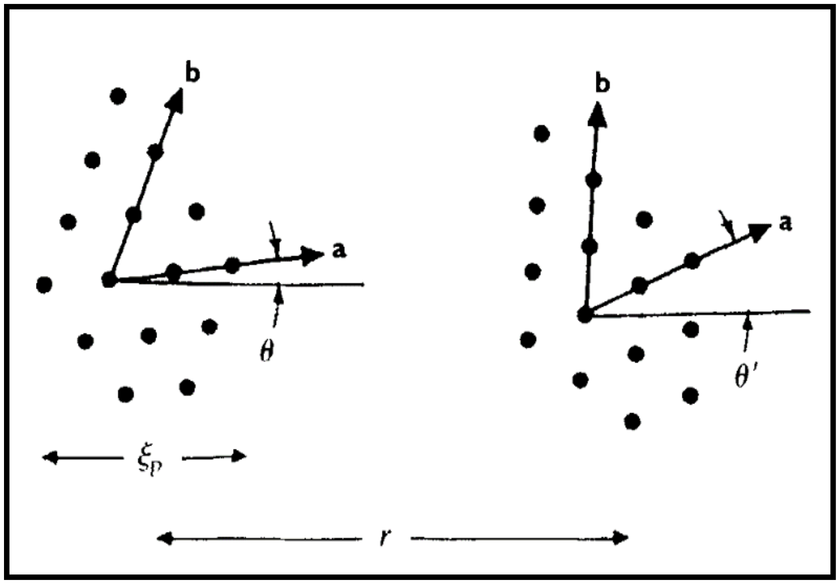
- Elongated organic molecules form equidistant layers
- In-plane structure of each layer:
  - Smectic (Sm-A) – liquid-like (short-range order)
  - Crystal (Cr-E or Cr-B) – long-range order
  - Hexatic (Hex-B) – short-range positional and long-range orientational order



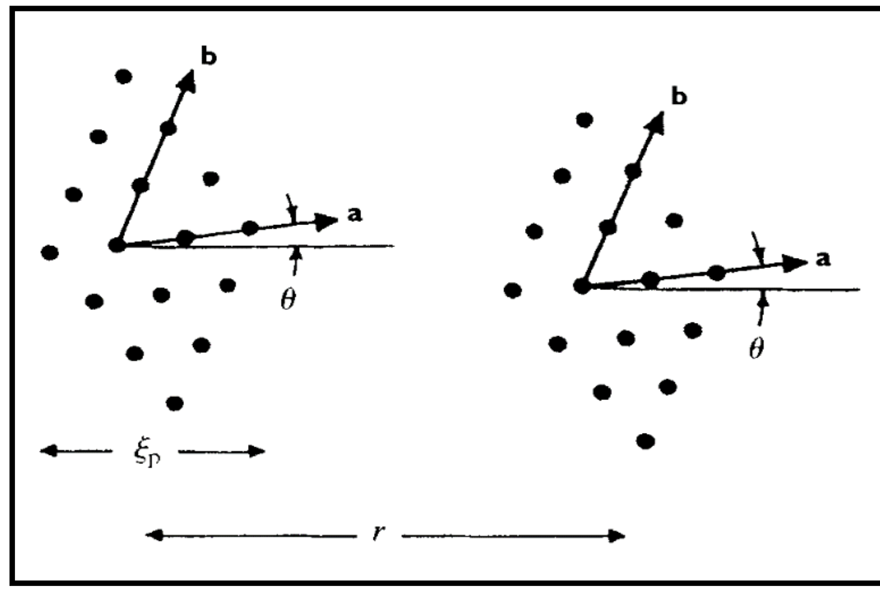
*B. Halperin and D. Nelson, PRL, **41**, 121, (1978)*

Bond-orientational order and hexatic phase

Smectic A: positional and BO short-range order.

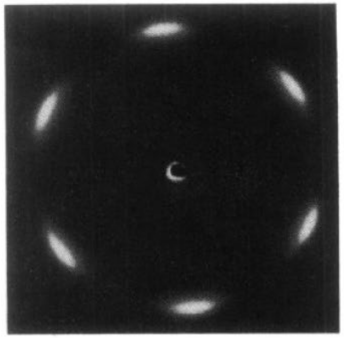


Hexatic B: short-range positional, and long-range BO order.



J.D. Brock, *et al.*, Contemporary Physics **30**, 321 (1989)

Scattering from hexatic phase



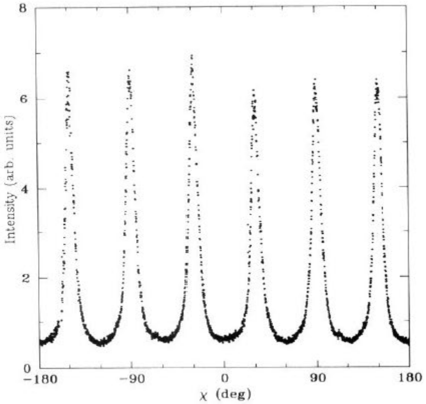


Fig. 2. X-ray diffraction pattern of hexatic membrane and corresponding χ scan

Fourier expansion of the azimuthal scattering profile:

$$I(\varphi) = I_0\left[\frac{1}{2} + \sum_{m=1}^{\infty} C_{6m} cos(6m(\varphi - \varphi_0))\right]$$

In the previous studies fitting procedure was used to determine Fourier components of intensity C_{6m}

Multicritical scaling theory (MCST)

In the frame of the MCST the BO parameters:

$$C_{6m} = [C_6]^{\sigma_m}$$

With exponent σ_m:

$$\sigma_m = m + x_m \cdot m(m-1)$$

where:

$$x_m \cong \lambda - \mu m + \nu m^2$$

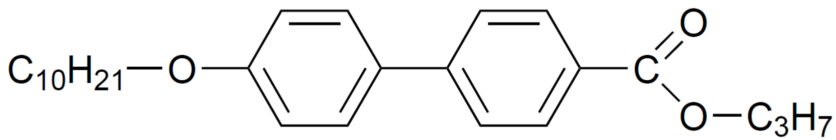
Theory predicts that:

$\lambda=1$ → 2D case

$\lambda=0.3$ → 3D case

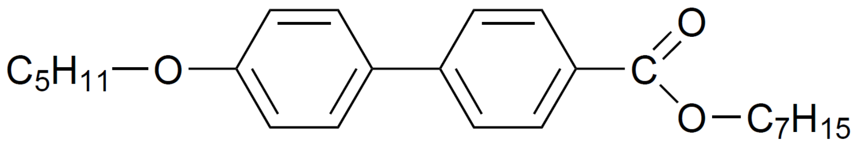
Samples

3(10)OBC:



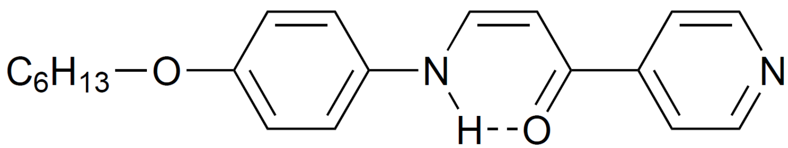
Sm-A $\xrightarrow{66.3\ ^\circ C}$ Hex-B $\xrightarrow{54.0\ ^\circ C}$ Cr-E

75OBC:

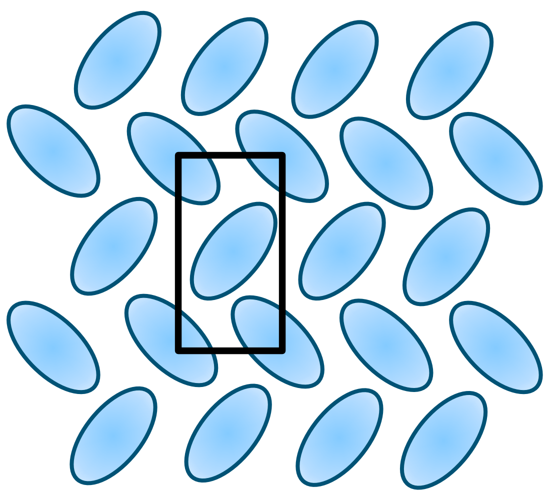


Sm-A $\xrightarrow{63.8\ ^\circ C}$ Hex-B $\xrightarrow{59.0\ ^\circ C}$ Cr-E

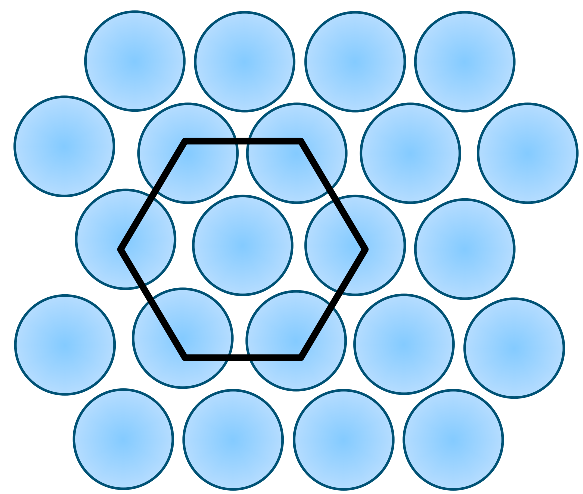
PIRO6:



Sm-A $\xrightarrow{92.6\ ^\circ C}$ Hex-B $\xrightarrow{85.0\ ^\circ C}$ Cr-B



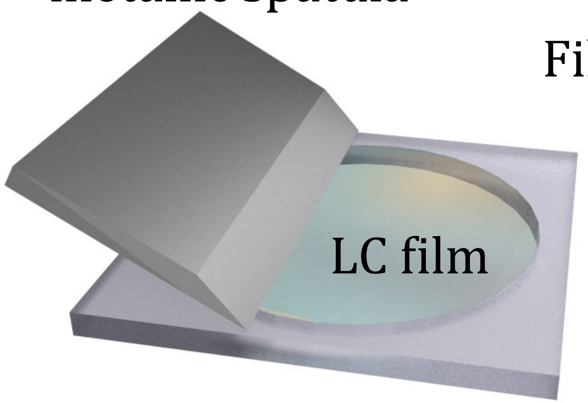
Cr-E



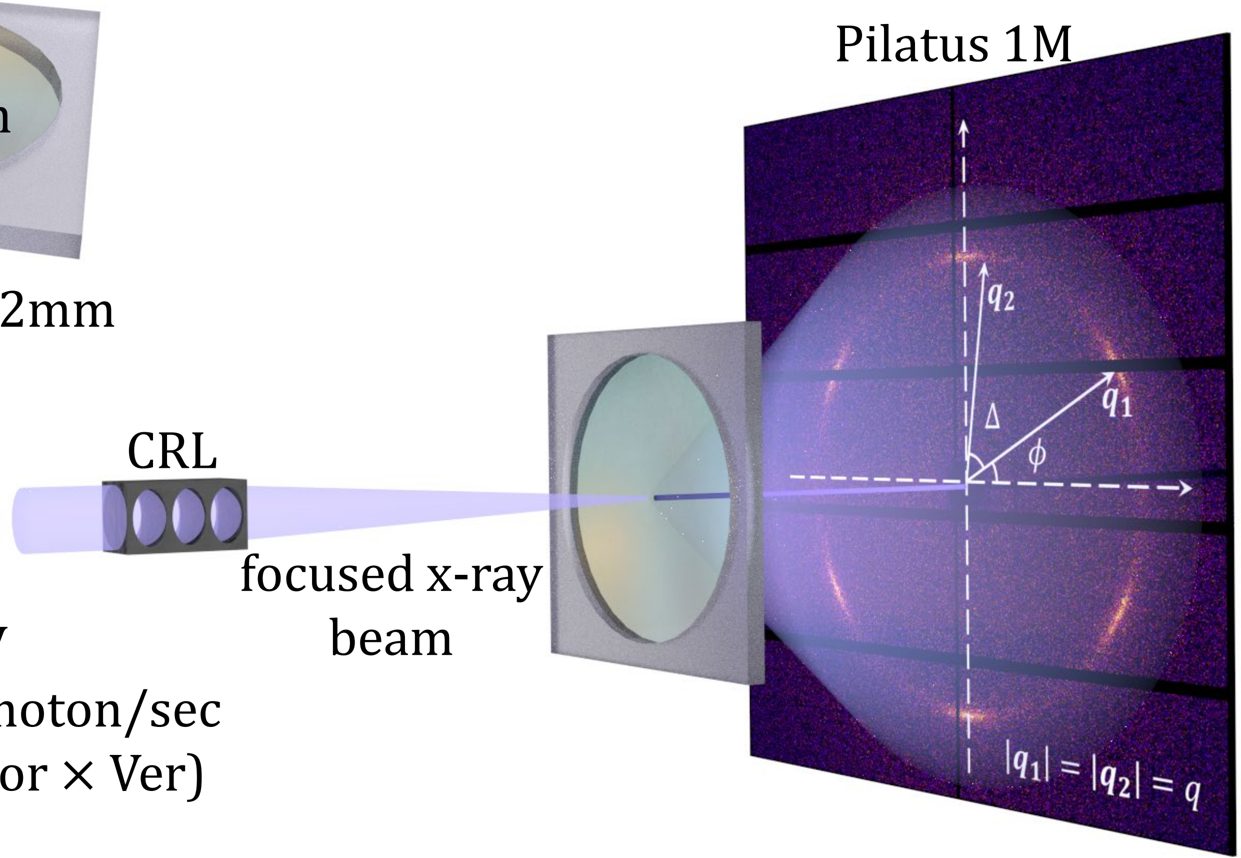
Cr-B

I. Zaluzhnyy *et al.*, Soft Matter **13**, 3240 (2017)

X-ray diffraction experimenta at P10 beamline (PETRA III)



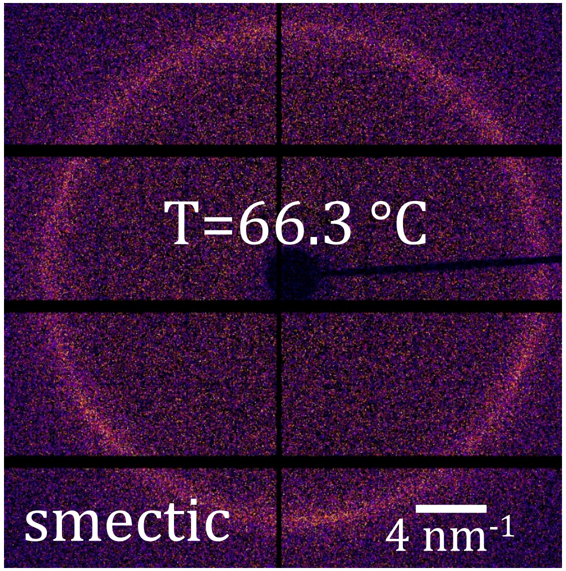
Film thickness: 5-7 μm (2-3 × 10^3 molecular layers)

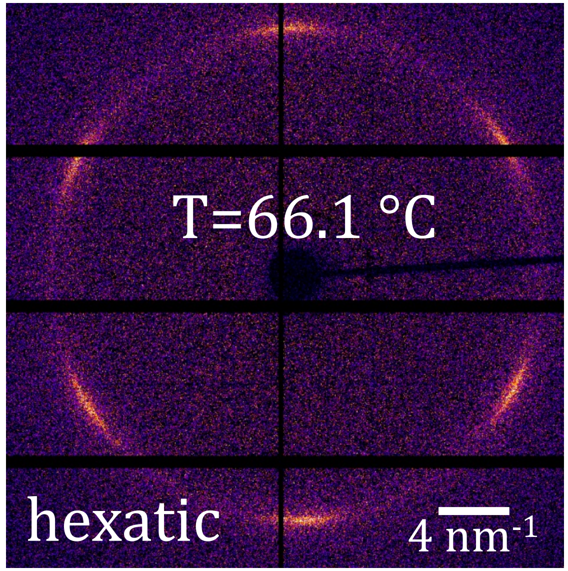


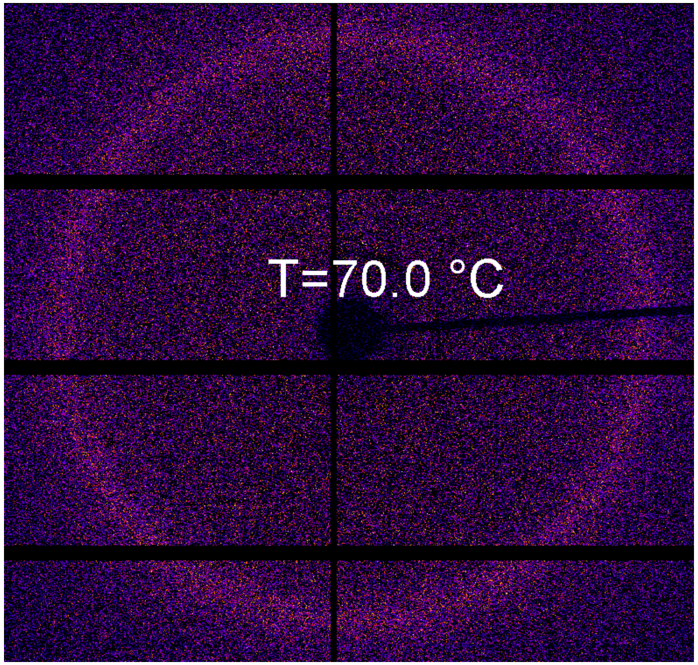
Energy: $E = 13.0$ keV
Flux: $F \sim 3 \cdot 10^{10}$ photon/sec
Beam size: 3×2 μm^2 (Hor × Ver)
Exposure: $\Delta t = 0.6$ sec

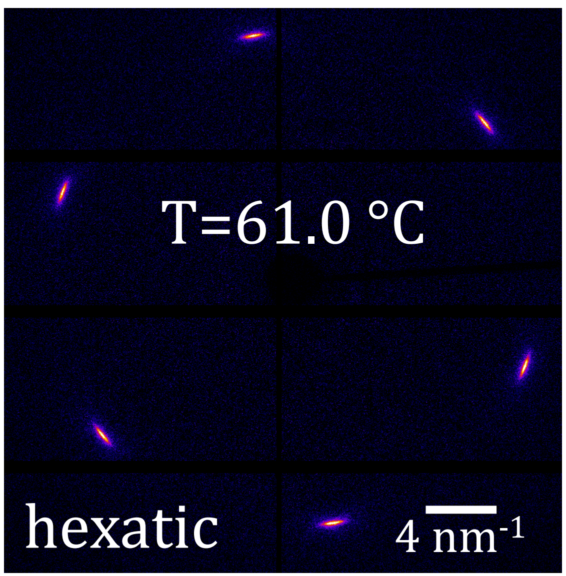
*I. Zaluzhnyy et al., PRE, **91**, 04256, (2015)*

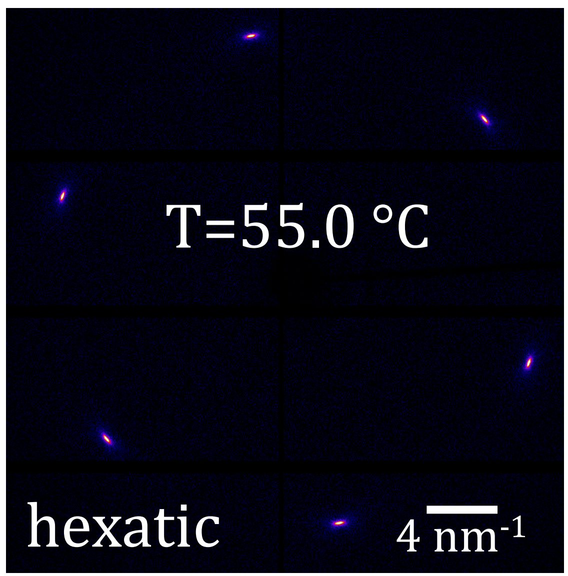
Measured diffraction patterns



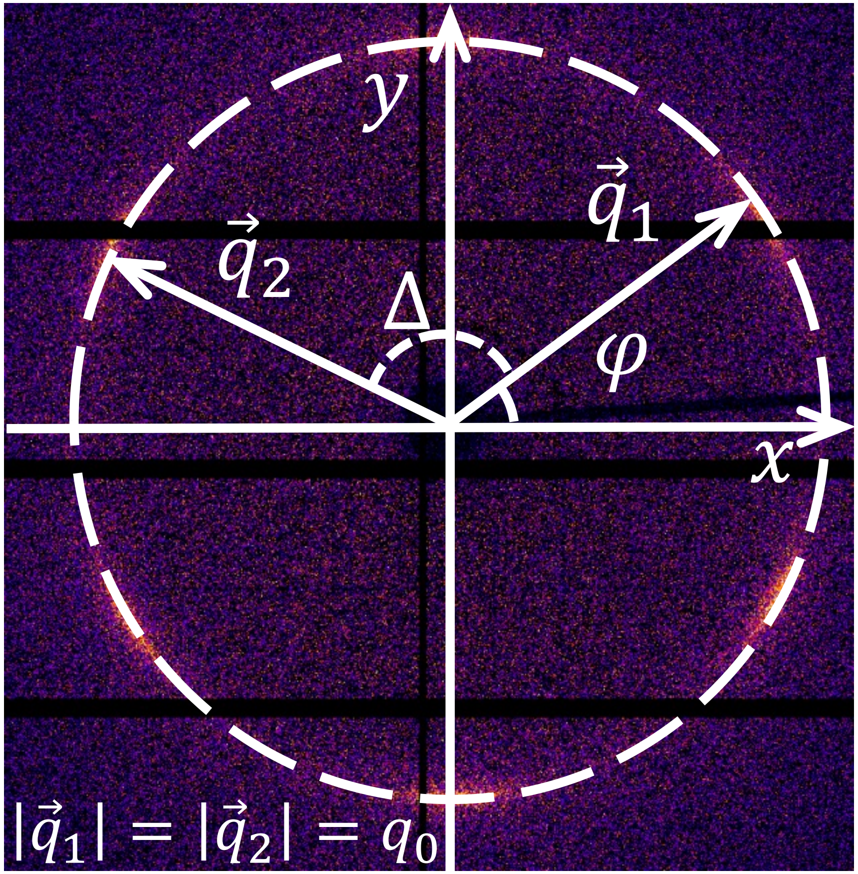








XCCA: two-point cross-correlation function (CCF)



- CCF calculation

$$C(q,\Delta) = \langle I(q,\varphi) I(q,\varphi+\Delta)\rangle_\varphi$$

- Fourier coefficients of the CCF

$$C(q,\Delta) = C_0(q) + 2\sum_{n=1}^{n=+\infty} C_n(q)\cos(n\Delta)$$

$$\langle C_n(q)\rangle_M = |I_n(q)|^2$$

- Averaging

$$\langle C_n(q)\rangle_M = \frac{1}{M}\sum_{m=1}^{M}\{C_n(q)\}^m$$

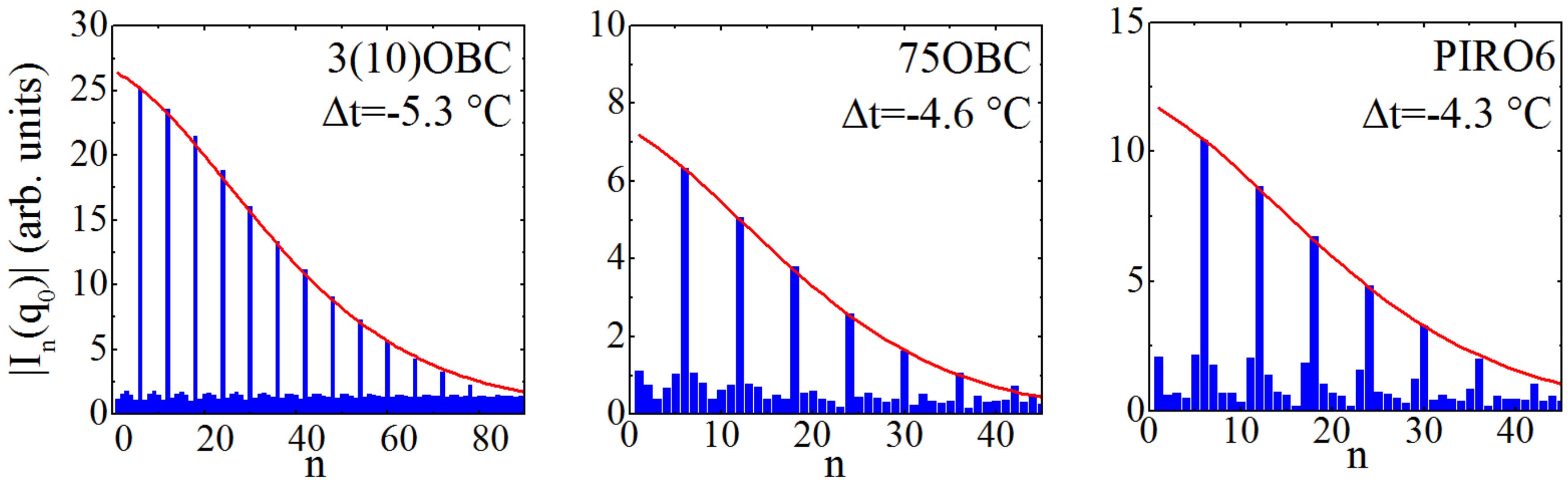
By applying XCCA analysis Fourier components of intensity $I^n(q)$ can be determined directly from diffraction patterns

R. Kurta et al., Adv. Chem. Phys. ***161****, (2016)*

Bond-orientational order

> Angular Fourier components of intensity

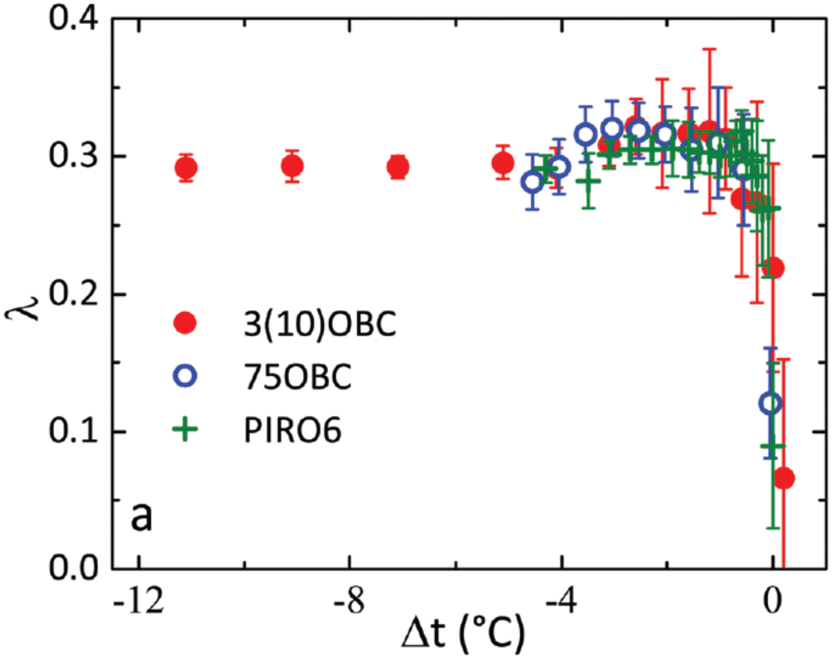
$$I_n(q) = \frac{1}{2\pi}\int_0^{2\pi} I(q,\varphi)e^{-in\varphi}d\varphi$$



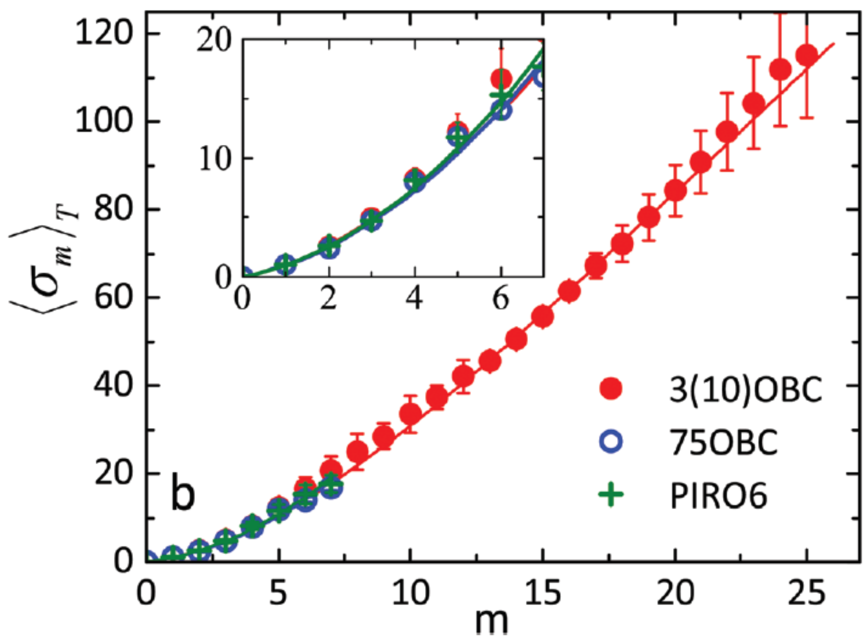
> The bond-orientational (BO) order parameters: $C_{6m} = \left|\frac{I_{6m}(q_0)}{I_0(q_0)}\right|$

> Red curve – prediction of MCST

Bond-orientational order



Temperature dependence of the parameter λ



Temperature averaged values of $<\sigma_m>_T$

3(10)OBC:	75OBC:	PIRO6:	Indication:
λ=0.31 μ=0.009	λ=0.27	λ=0.29	3D case

Angular correlations in mesocrystals studied with nanodiffraction

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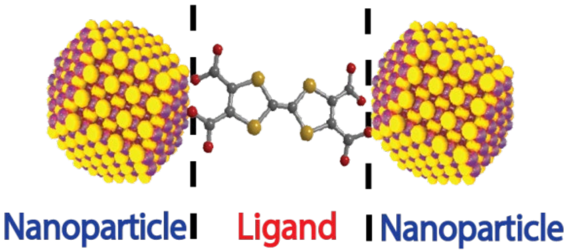
I. Zaluzhnyy *et al.*, Nano Lett. **17**, 3511 (2017)
N. Mukharamova *et al.*, Small **15,** 1904954 (2019)

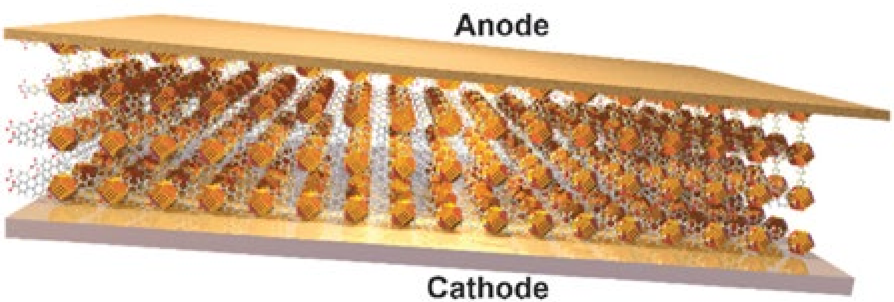
Coupled organic-inorganic nanostructures (COIN)

Hybrid nanostructures are coupled in two ways:

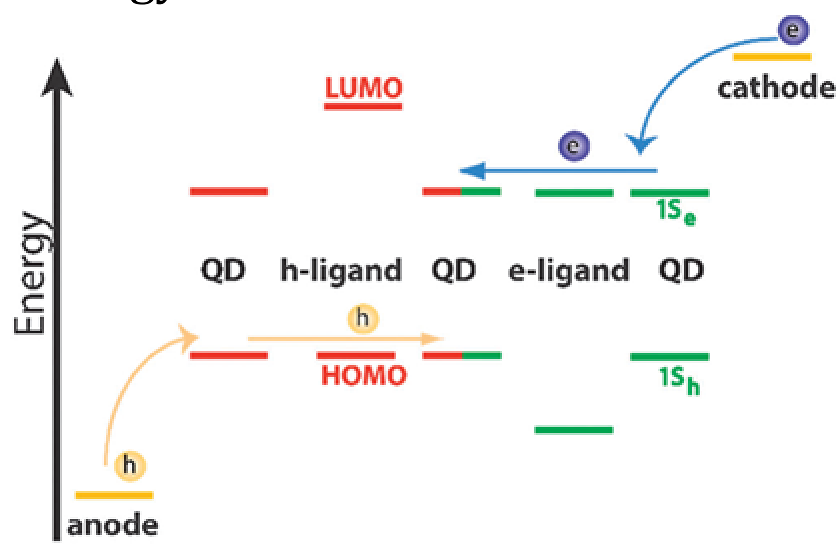
- electronically via potentially near-resonant alignment of suitable energy levels
- chemically through a strong binding interaction.



A diode composed of a COIN bilayer sandwiched in between an anode and a cathode



Energy scheme of a COIN diode

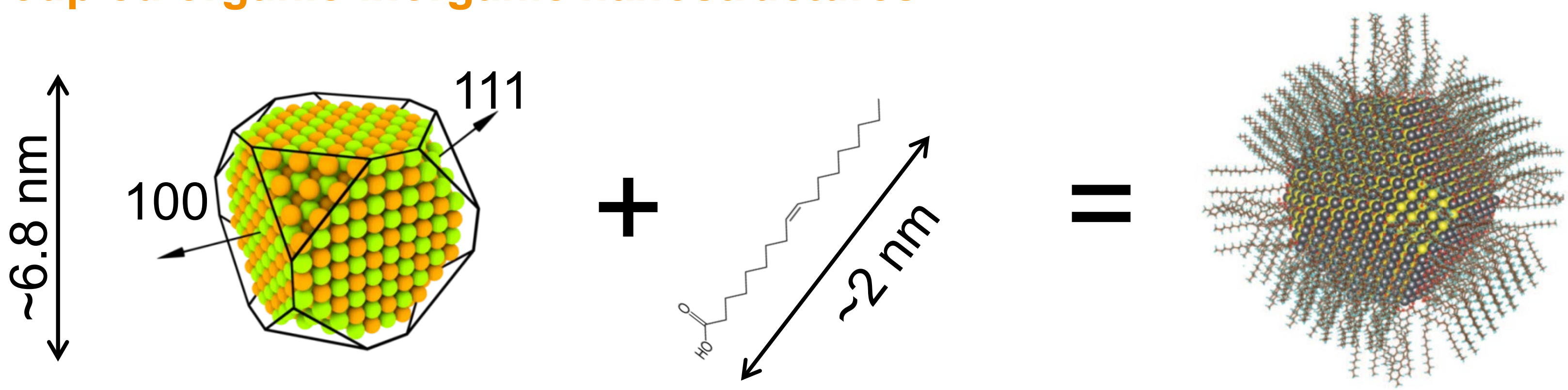


M. Scheele et al., Phys. Chem. Chem. Phys. **17**, 97 (2015)

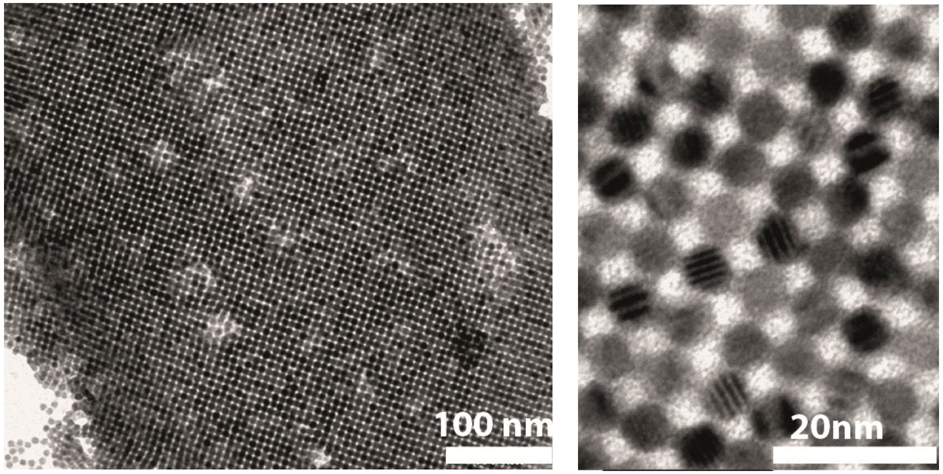
Mesocrystalline structures

The notation "mesocrystal" is an abbreviation for a mesoscopically structured crystal, which is an ordered superstructure of crystals with mesoscopic size (1–1000 nm).

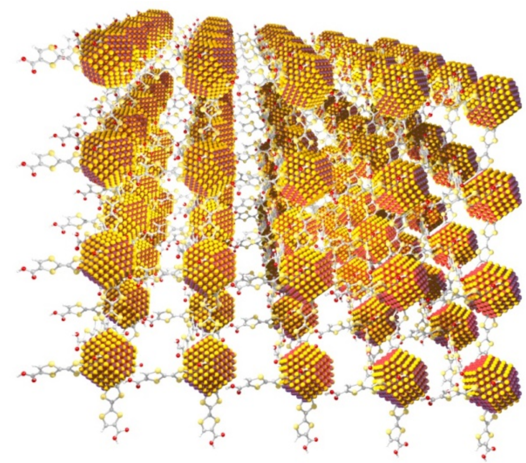
Coupled organic-inorganic nanostructures



TEM of PbS nanocrystals



Nanocrystal superlattice



Previous study:
Zaluzhnyy, Ivan A., et al. Nano letters 17.6 (2017): 3511-3517.

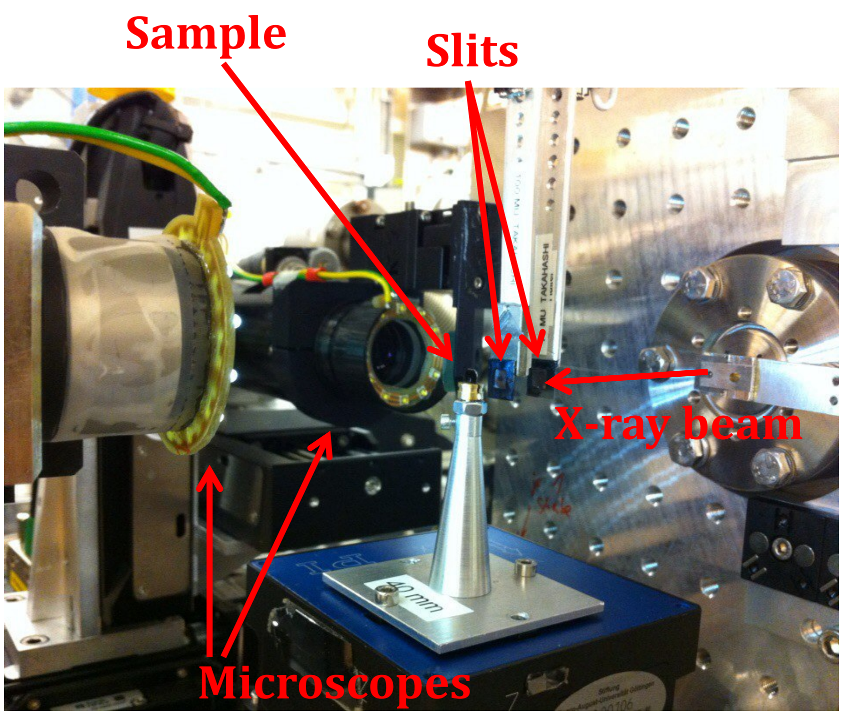
Experimental setup

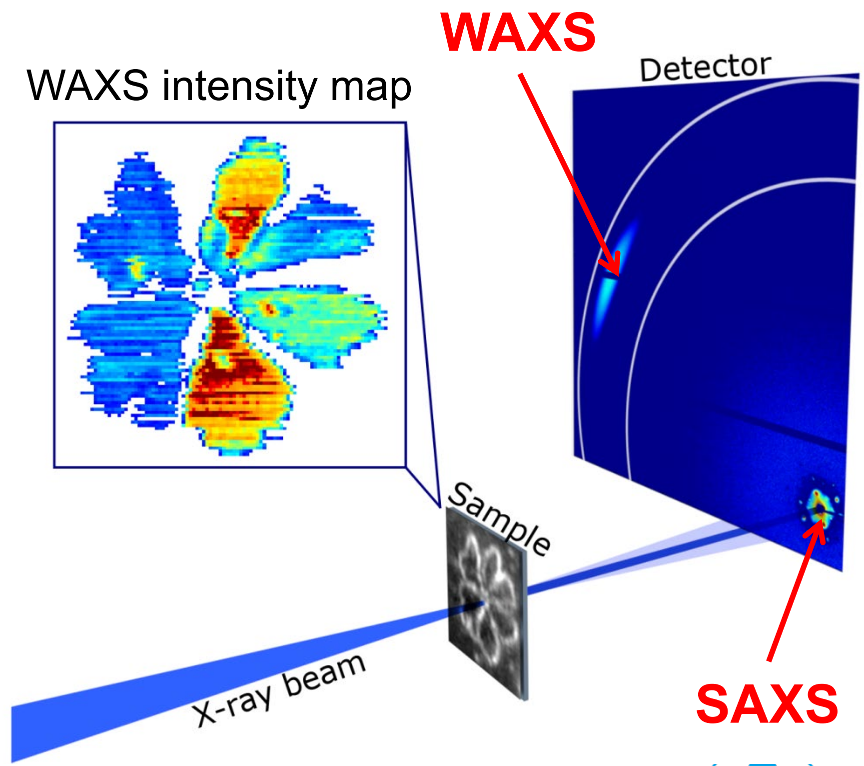
P10 beamline, PETRA III (GINIX setup)

X-ray beam:
E = 13.8 keV
Size = 400x400 nm^2
Flux = 10^{10}-10^{11} ph/sec

Detector Eiger 4M
Size = 2070x2167 pixels
Pixel size = 75x75 μm
SDD= 41 cm

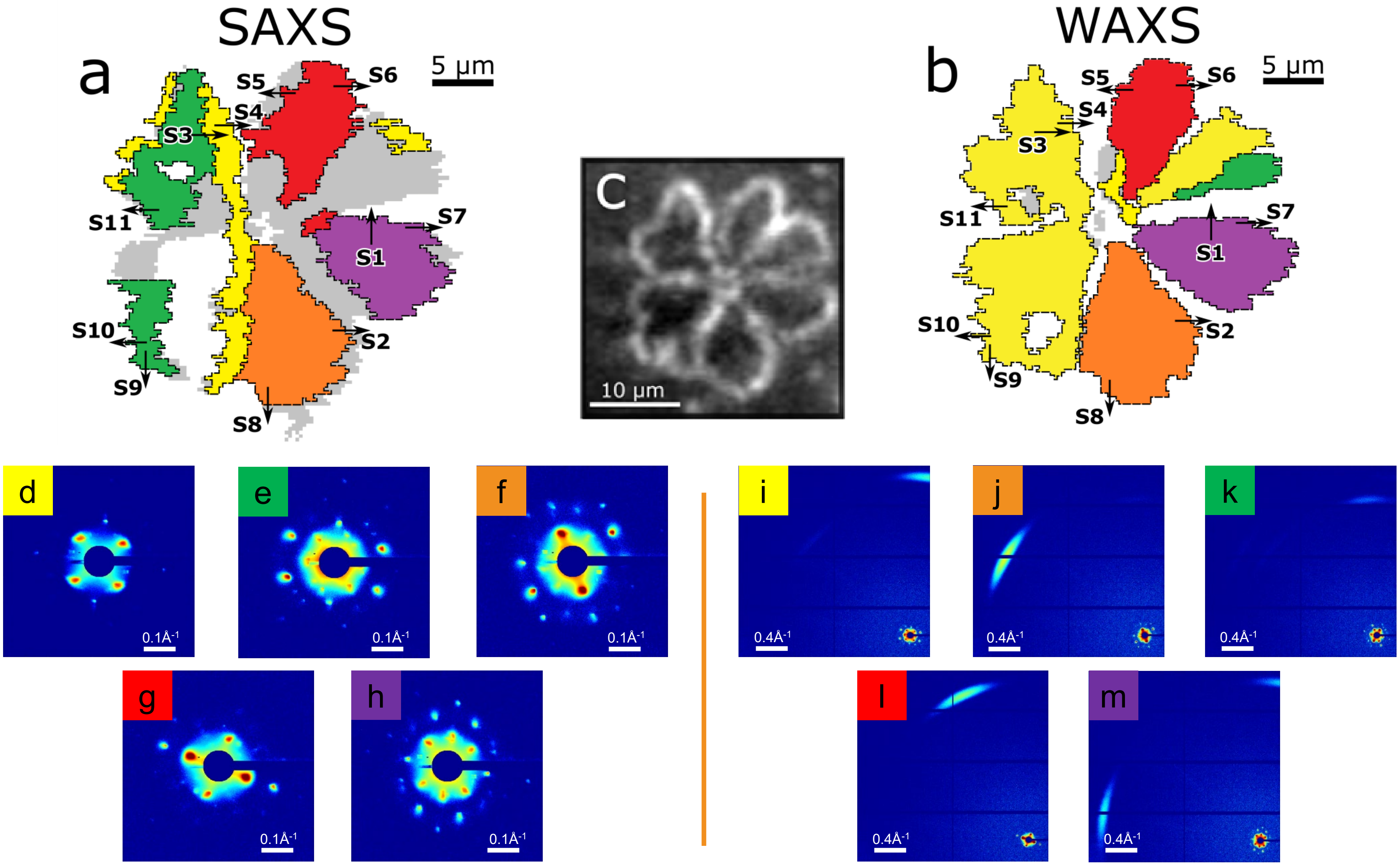
Spatial scanning:
121x121 points with 250 nm step size.
Substrate:
Si_3N_4-membrane,
0.5x0.5 mm^2, 50 nm thick





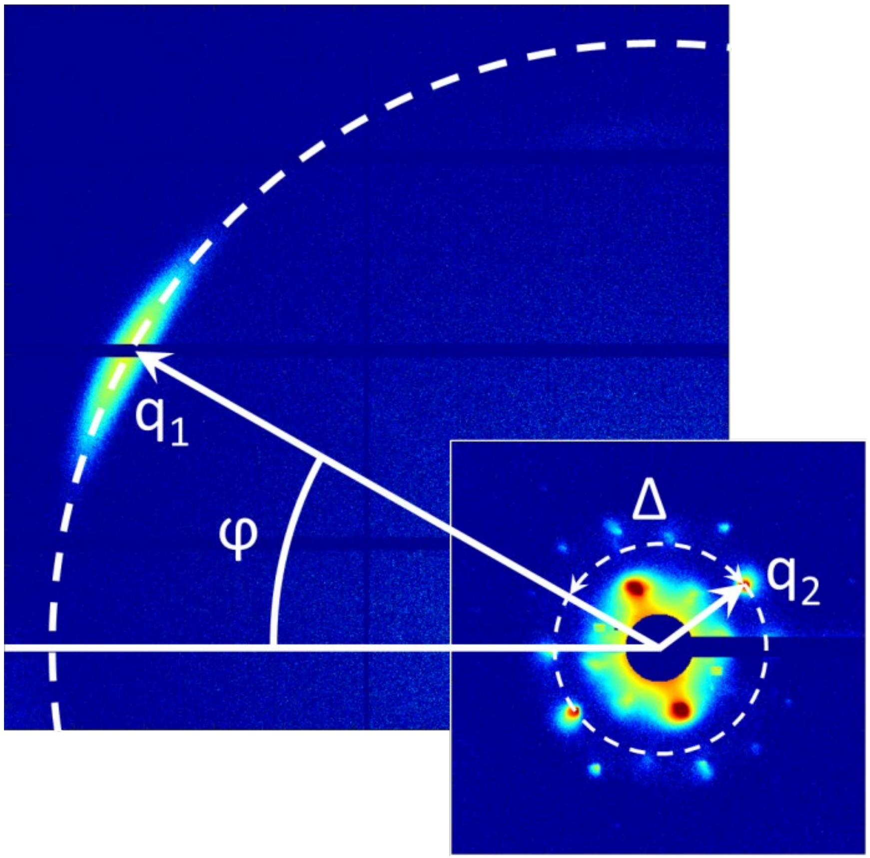
Spatial diffraction maps

Domain structure with different orientations of SL and AL



Cross-Correlation Analysis

WAXS



SAXS

> CCF calculation

$$C(q_1,q_2,\Delta) = \frac{1}{2\pi}\int_{-\pi}^{\pi} I(q_1,\varphi)I(q_2,\varphi+\Delta)d\varphi$$

$$= \int_{-\pi}^{\pi} I(q_1,\varphi)W(q_1,\varphi)I(q_2,\varphi+\Delta)W(q_2,\varphi+\Delta)d\varphi$$

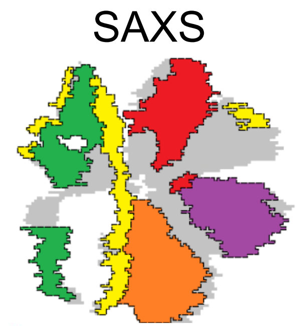
> Mask

$$W(q,\varphi) = \begin{cases} 0, & \text{gaps, beamstop, detector edges} \\ 1, & \text{otherwise} \end{cases}$$

> Averaging

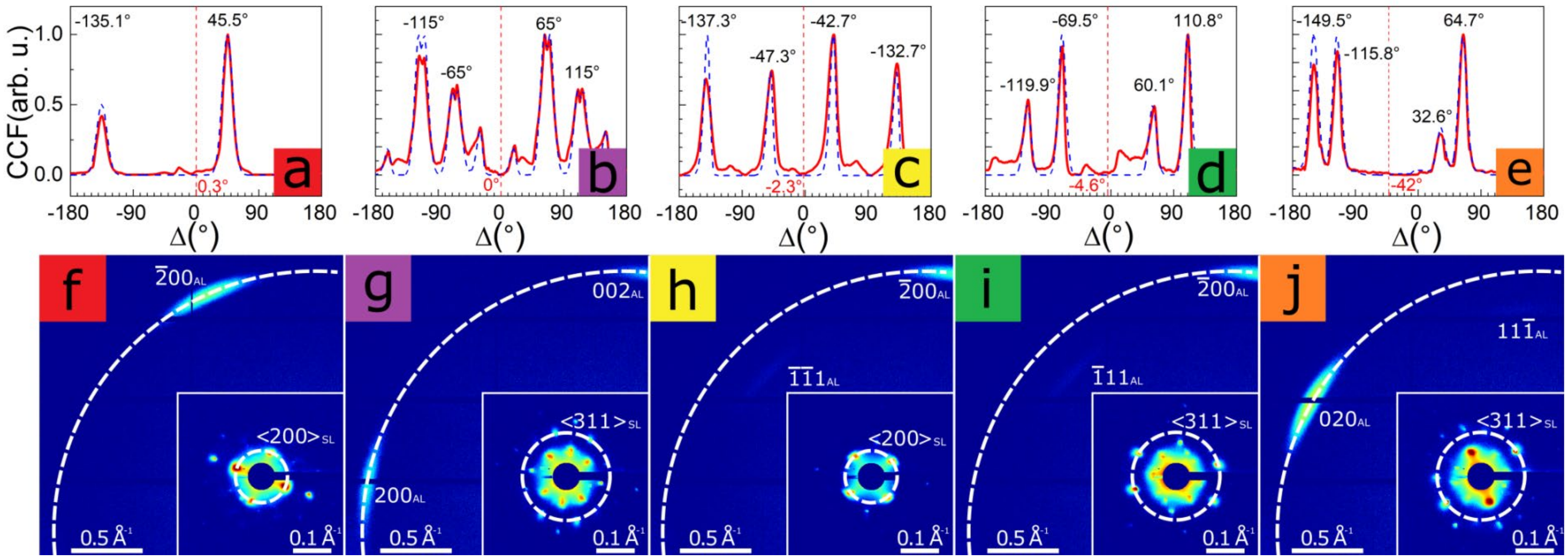
$$\langle C(q_1,q_2,\Delta)\rangle_M = \frac{1}{M}\sum_{i=1}^{M} C^i(q_1,q_2,\Delta)$$

Angular positions of NCs in SL

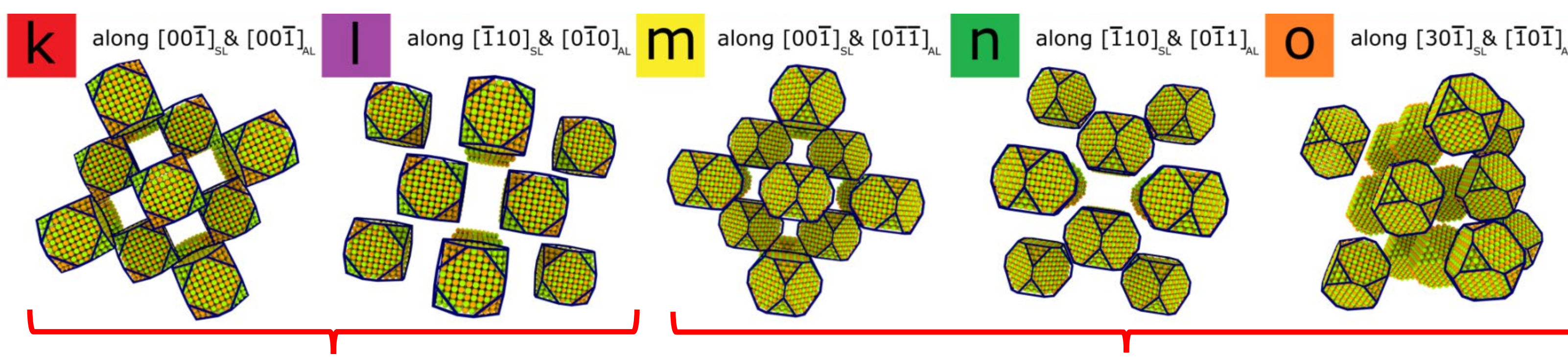


Resolved by XCCA

- Experimental (red) and simulated (blue) CCFs
- Correlated q-rings are shown by white dashed lines



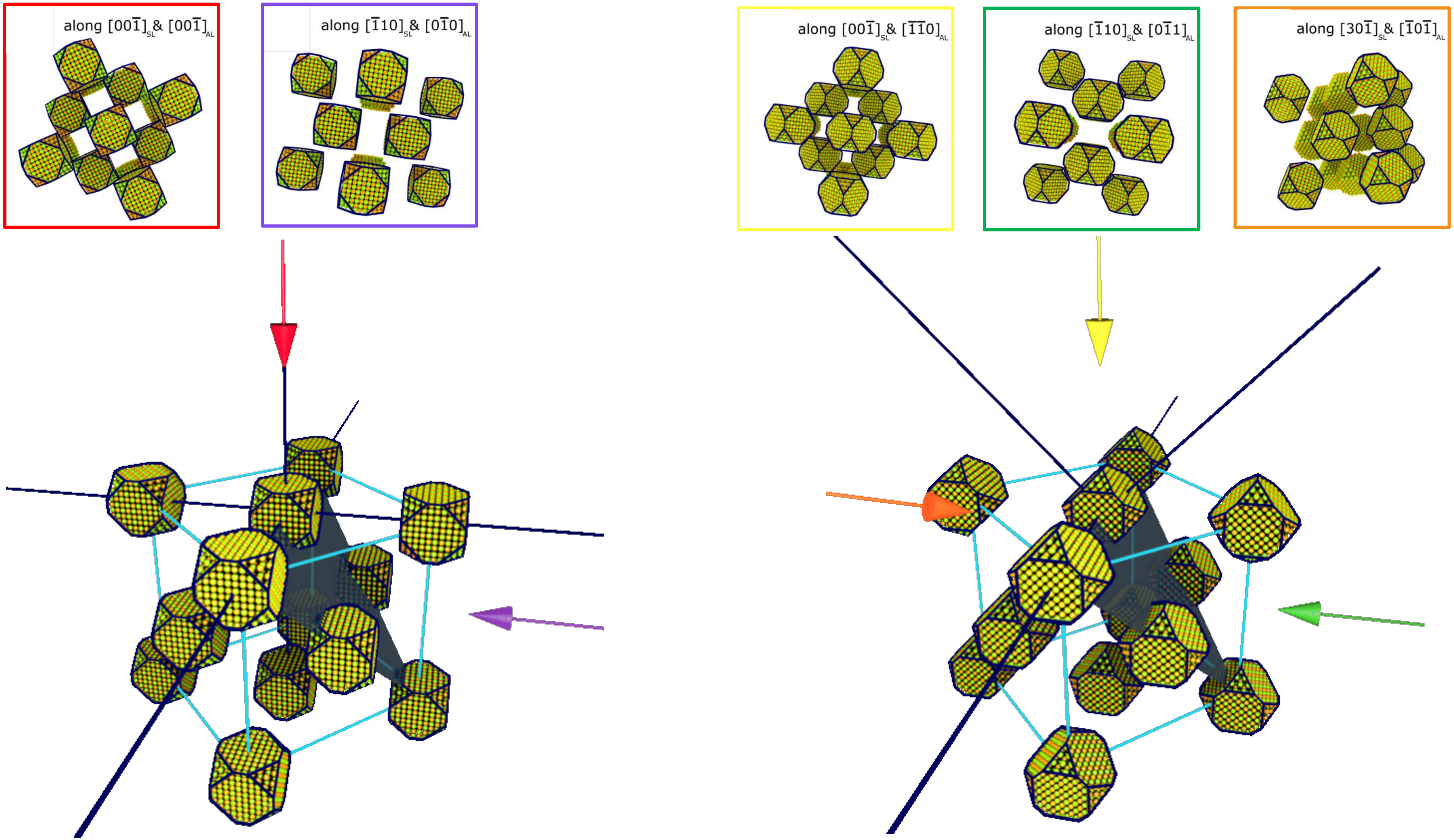
- Real space models of the superlattice and its constituting NCs



Configuration 1

Configuration 2

Two structural configurations

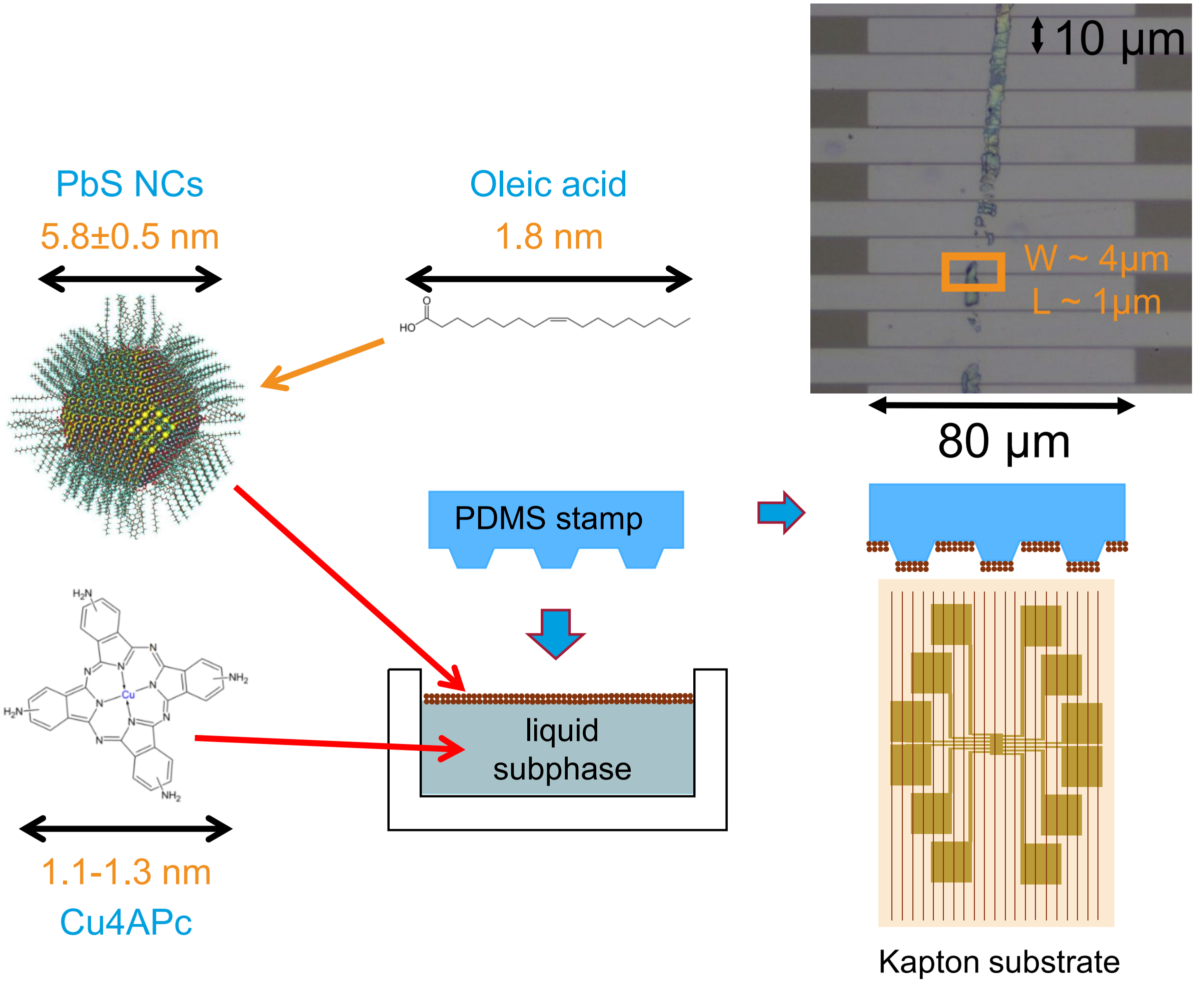


Anisotropic Charge Transport Revealed by Structure–Transport Correlations

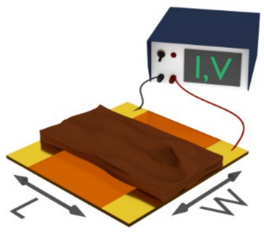
A. Maier *et al.*, Adv. Mater. **32,** 2002254 (2020)

PbS-Cu4APc mesocrystals

Ligand exchanged from PbS-OA

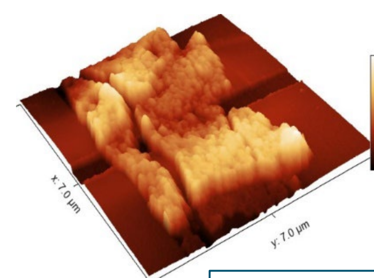


Conductivity measurements



conductance *G*

AFM map

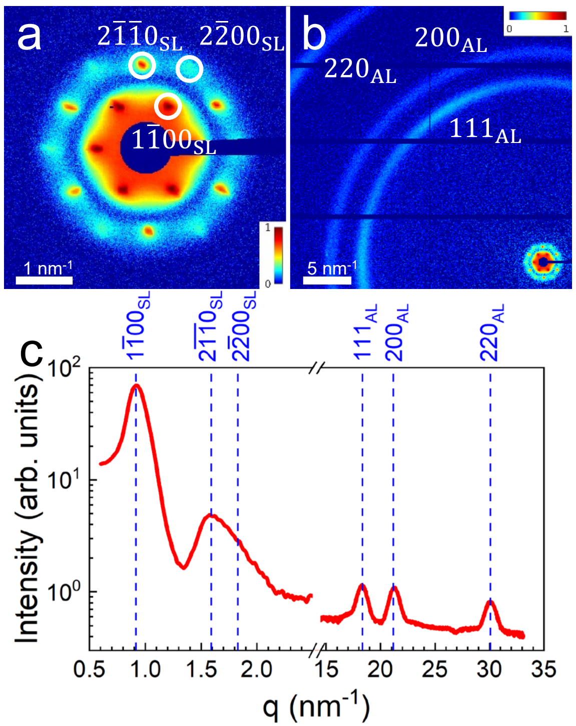


dimensions *L, W, h*

Two types of superlattice

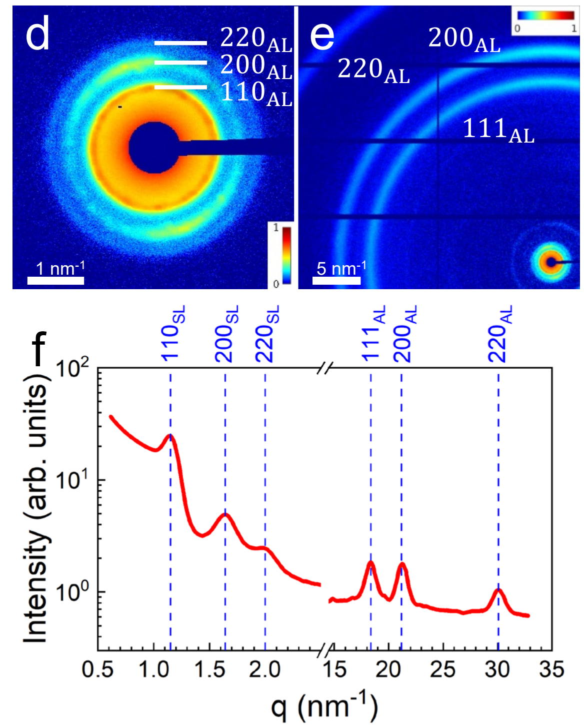
Monocrystalline rhcp

Oriented along $[0001]_{SL}$



Polycrystalline bcc

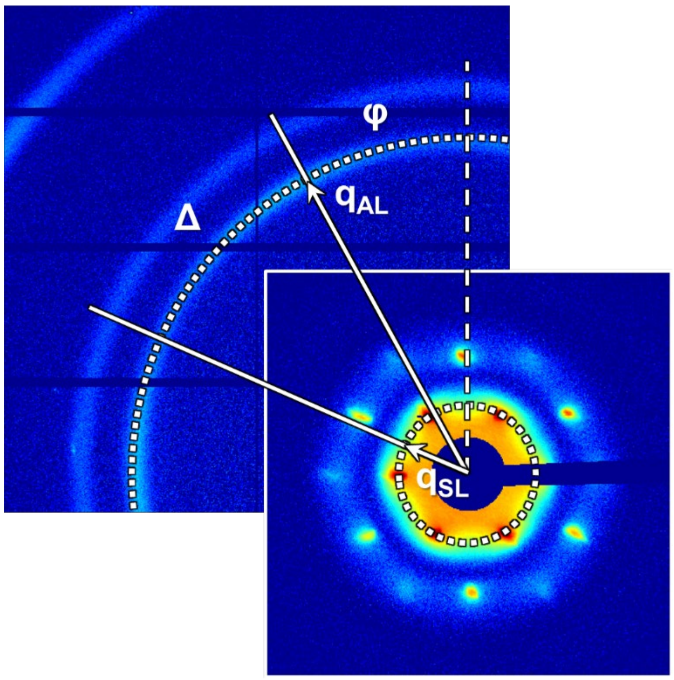
Oriented along $[110]_{SL}$



SAXS peak positions → SL unit cell parameter and nearest-neighbor distance

Angular X-ray Cross-Correlation Analysis

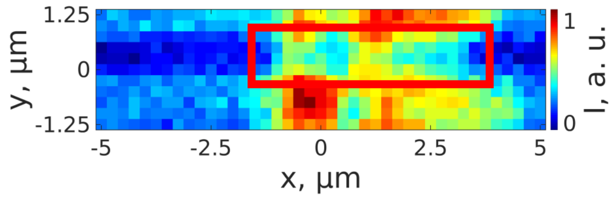
Basics



Cross-correlation function:

$$C(q_{AL}, q_{SL}, \Delta) = \frac{1}{2\pi} \int_{-\pi}^{\pi} I(q_{AL}, \varphi) I(q_{SL}, \varphi + \Delta) d\varphi$$

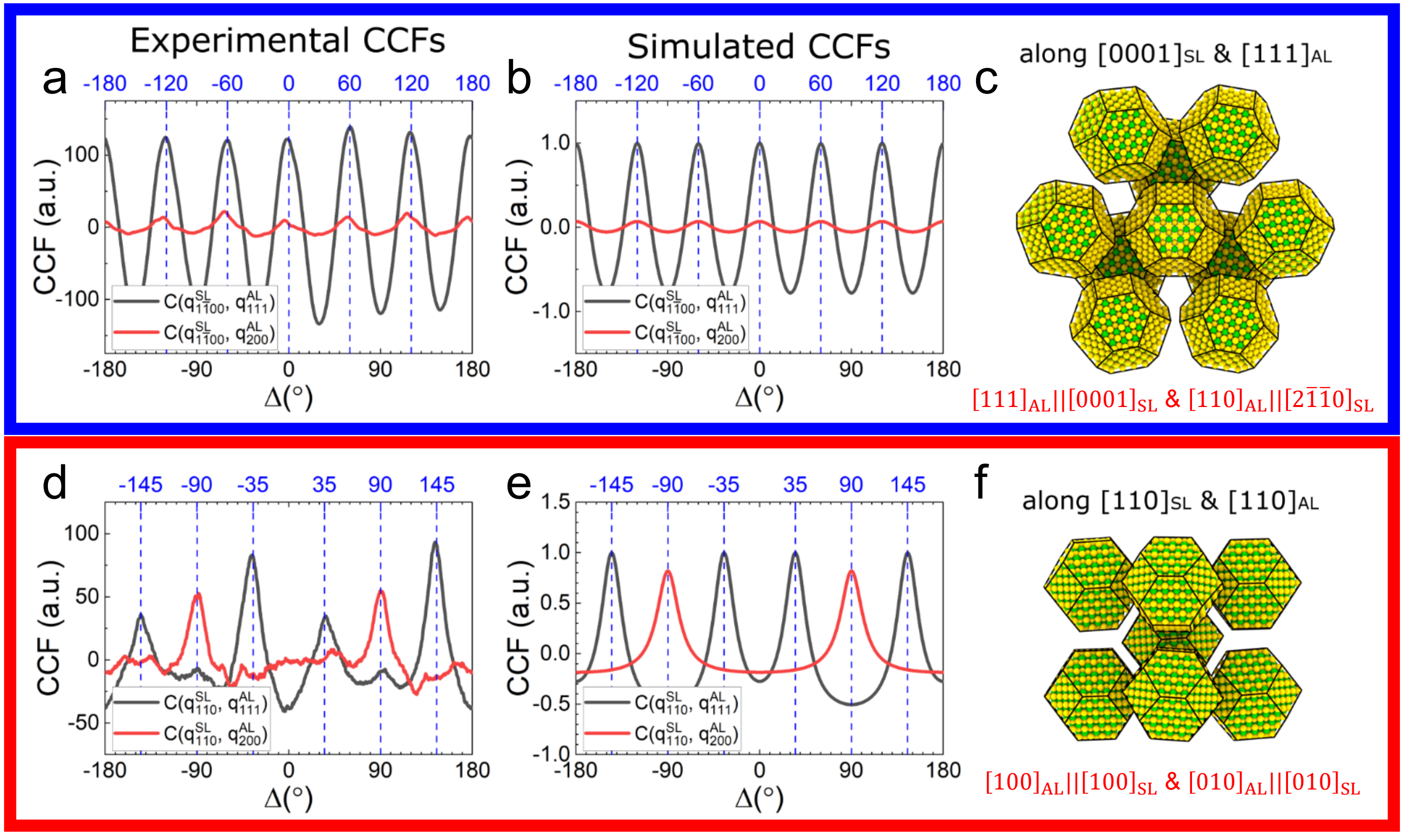
The cross-correlation functions are calculated for each diffraction pattern and then averaged over all patterns for each channel.



I.A. Zaluzhnyy et al. "Angular x-ray cross-correlation analysis (AXCCA): Basic concepts and recent applications to soft matter and nanomaterials." *Materials* 12.21 (2019): 3464.0

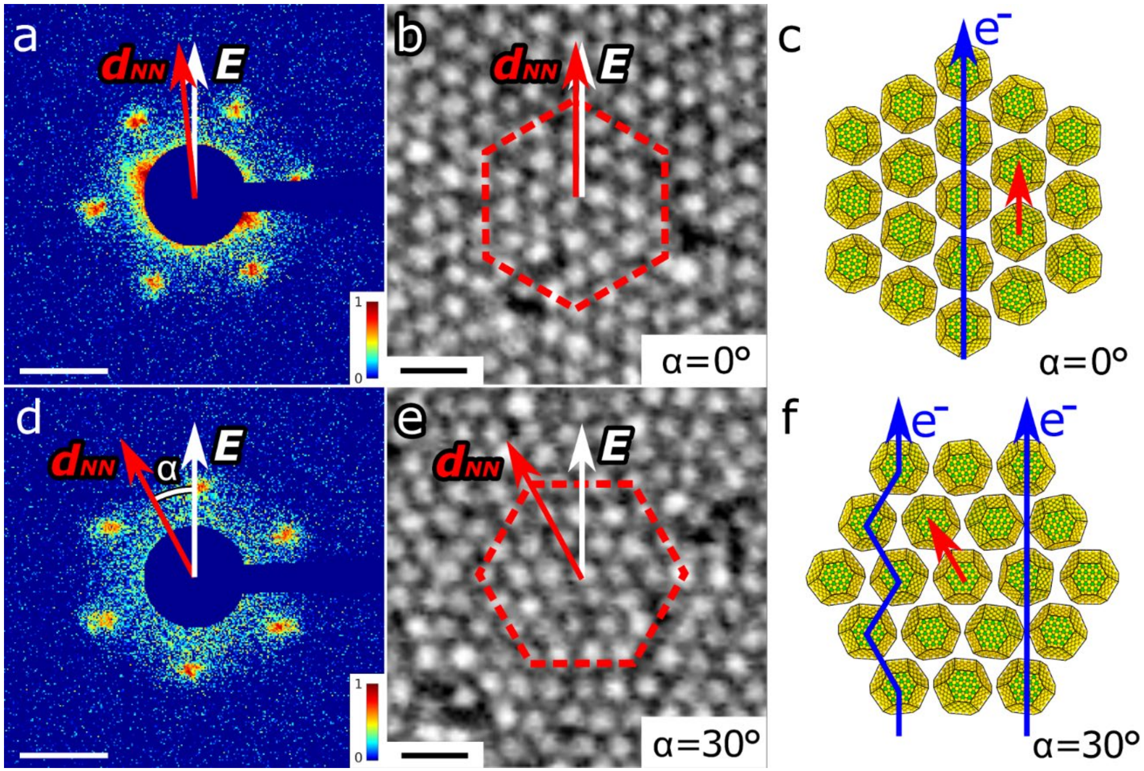
Angular X-ray Cross-Correlation Analysis

Reveals angular position of NCs in superlattice



Anistropy in conductivity

Observed for monocrystalline channels



When NCs are aligned along the field, the conductivity is higher by 40-50 %

The larger hopping distance or the zig-zag path are detrimental to charge transport

Determination of structural parameters of single crystalline grains with defects

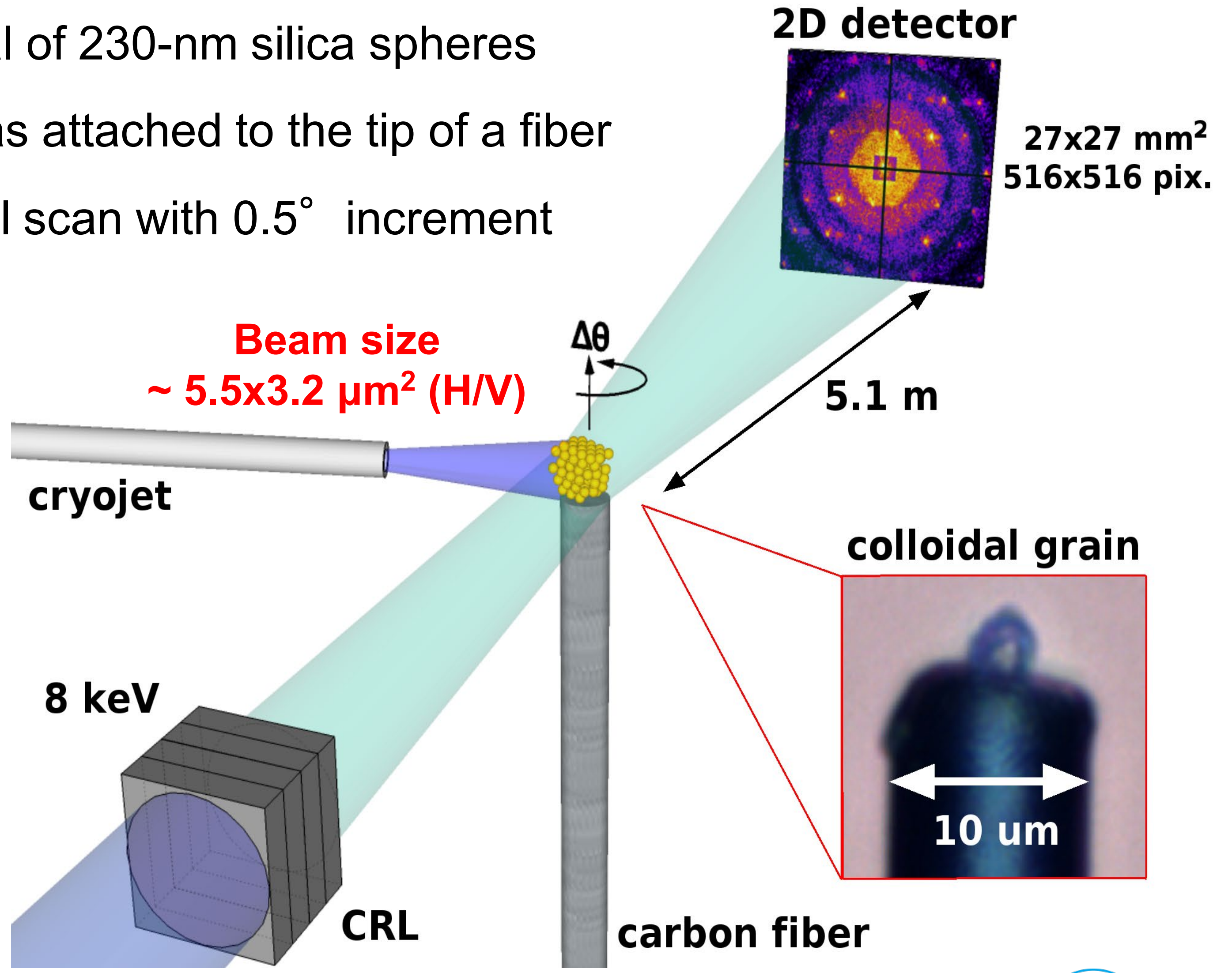
HELMHOLTZ
ASSOCIATION

DESY

D. Lapkin, *et al.*, (2021) (in preparation)

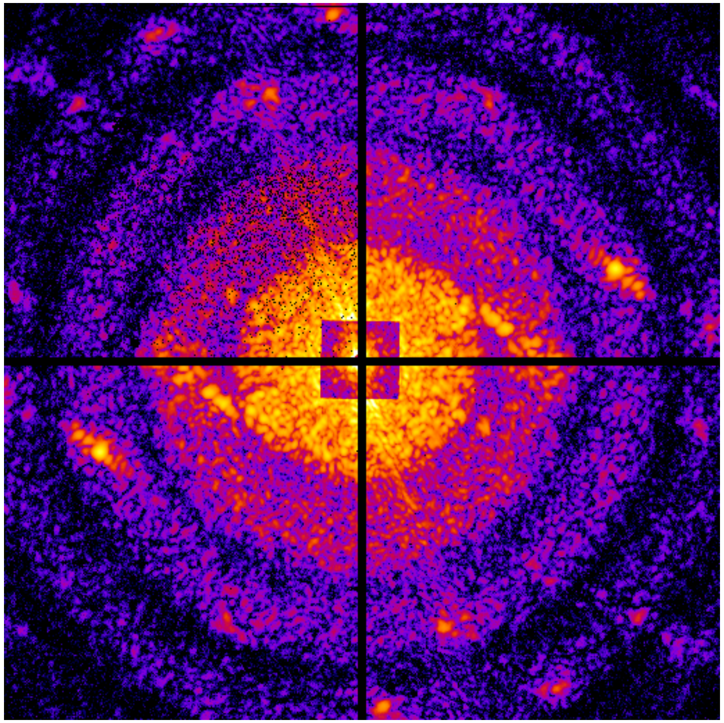
Experiment at P10 Beamline (PETRA III, DESY)

- Colloidal crystal of 230-nm silica spheres
- Single grain was attached to the tip of a fiber
- 180° azimuthal scan with 0.5° increment

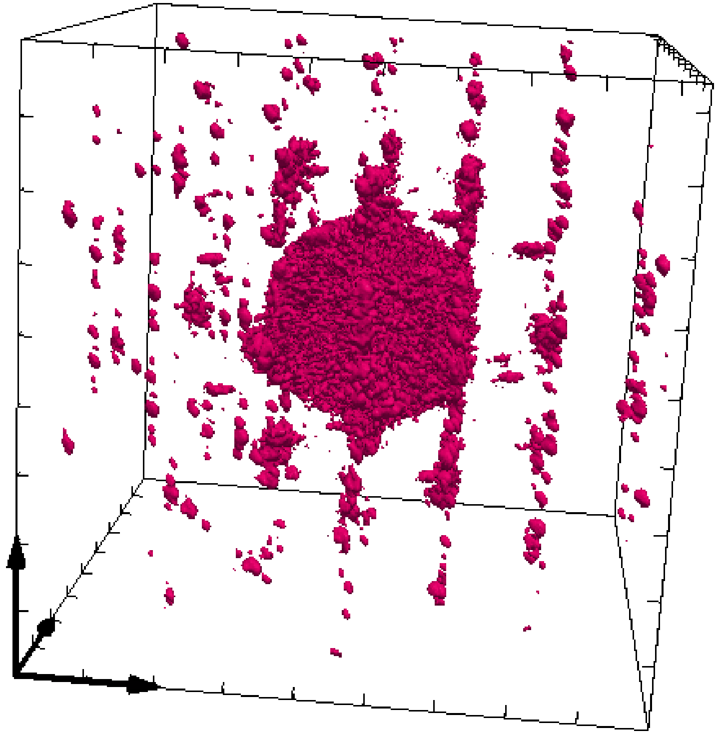


A. Shabalin, *et al.*, Phys. Rev. Lett. **117**, 138002 (2016)

Selected dataset: 180° rotation series with 0.5° increment



Diffraction patterns at different angles (360 images)



Stack of all images in 3D

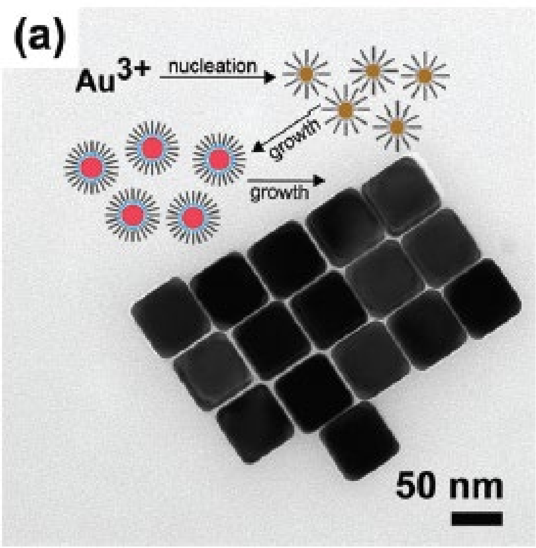
Determination of structural parameters of single crystalline grains

HELMHOLTZ | ASSOCIATION

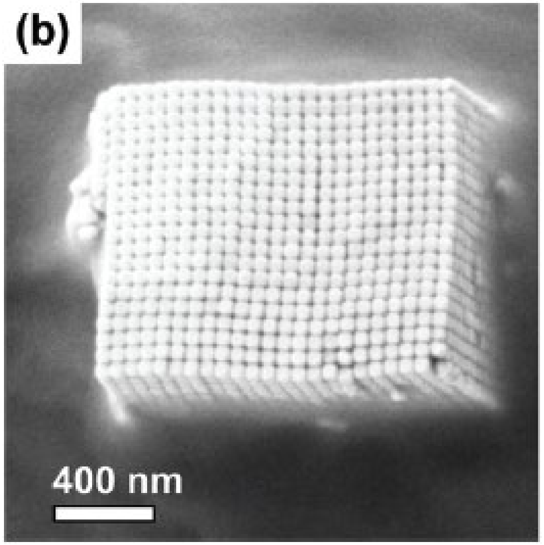
DESY

Experiment performed at LCLS

Synthesis of gold nanoparticles and mesocrystals



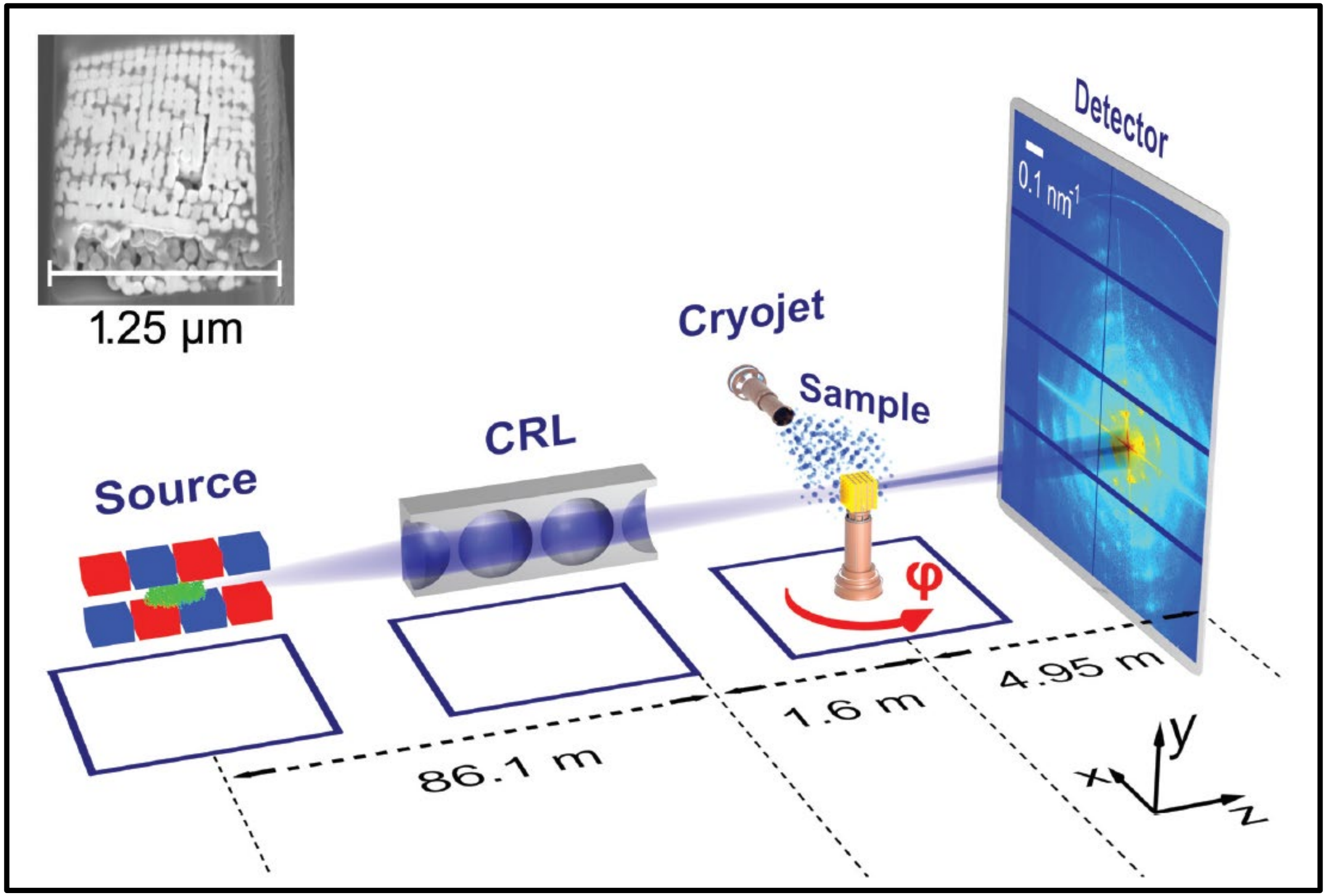
TEM image of gold nanocubes synthesized using a seed mediated approach



SEM image of the self assembled gold mesocrystal

Synthesis: group of E. Sturm (University of Konstanz)

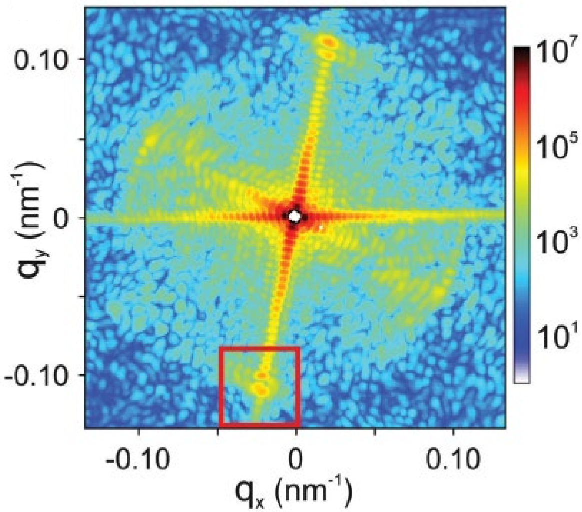
Experiment at PETRA III



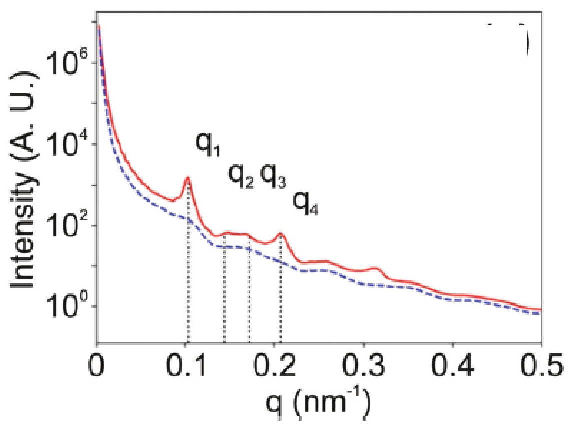
Schematic layout of the experiment performed at P10 beamline

J. Carnis *et al.*, Nanoscale (2021) DOI: 10.1039/d1nr01806j

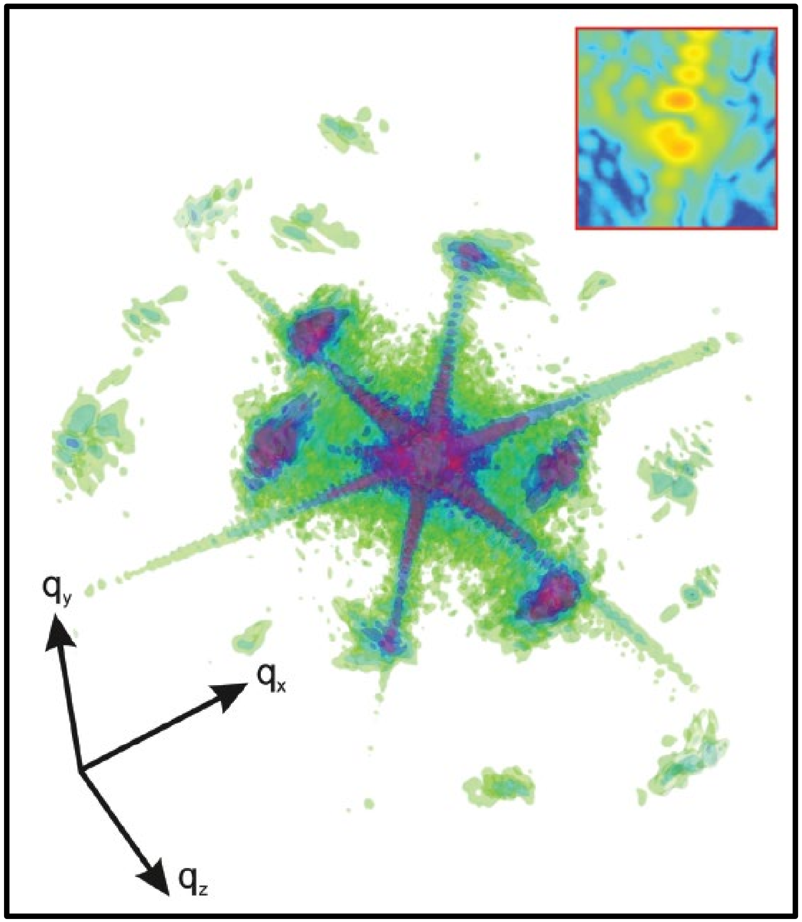
Experiment performed at PETRA III



Slice at the center of the diffraction pattern



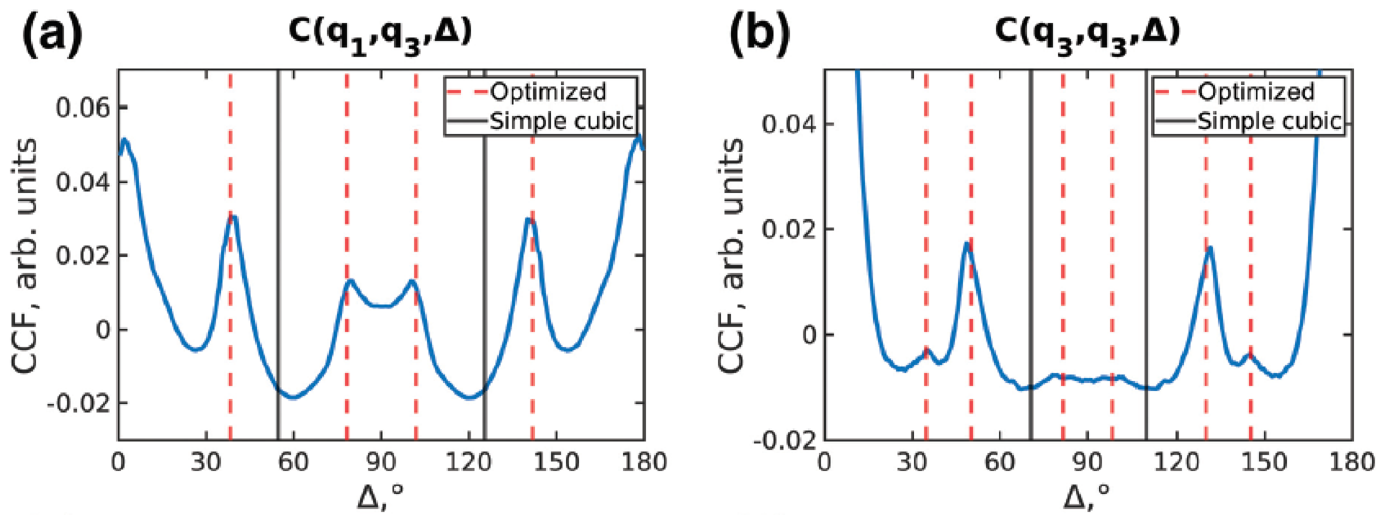
Intensity distribution as a function of *q* obtained by angular averaging of the 3D diffraction pattern

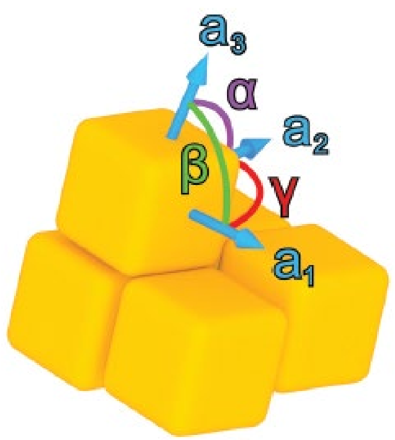


Isosurface view of the 3D diffraction pattern from the mesocrystalline grain

Angular X-ray Cross-Correlation Analysis

Angular X-ray cross-correlation functions (CCFs) $C(q_1,q_2,\Delta)$





Real space model of the superlattice

Optimized unit cell:

$a = b = 63.2$ nm,
$c = 62.2 \pm 0.1$ nm,
$\alpha = \beta = 75°$,
$\gamma = 90°$.

Ultrafast structural dynamics of photo-reactions

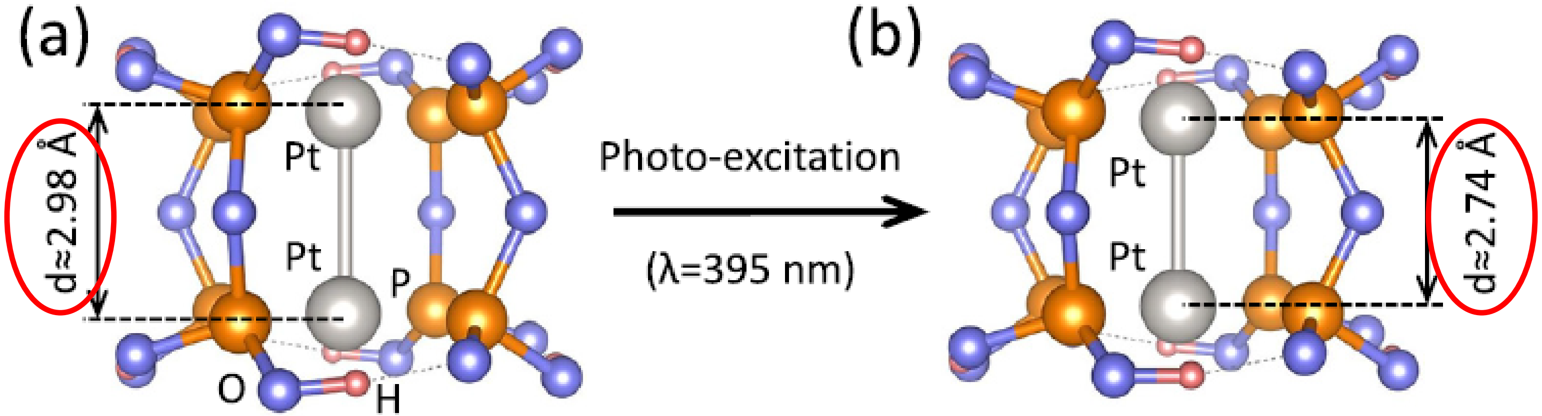
HELMHOLTZ
ASSOCIATION

DESY

P. Vester, *et al.*, Struct. Dyn. **6**, 024301 (2019)

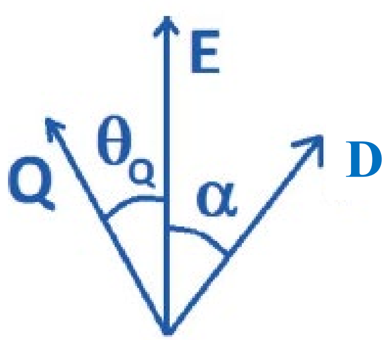
Experiment performed at LCLS

System: PtPOP molecule



Ground state

Excited state



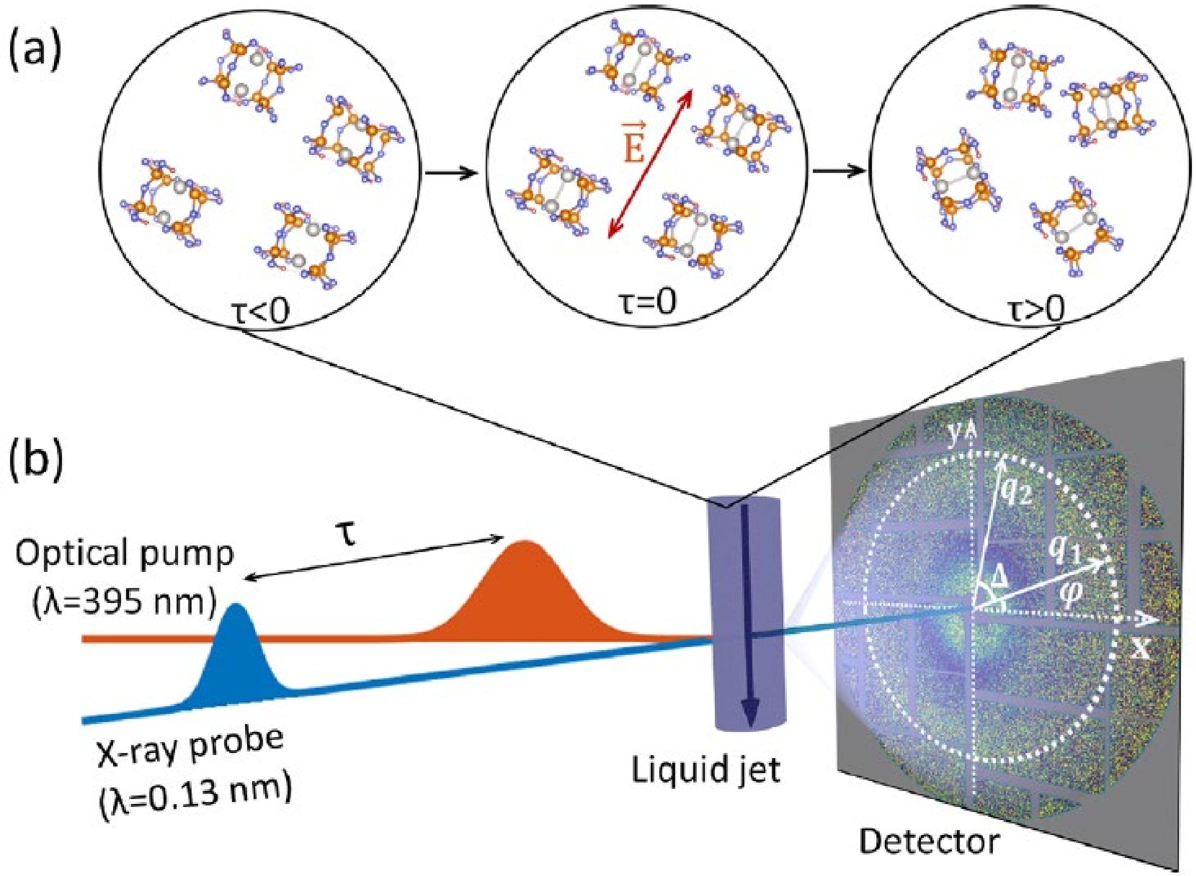
For one-photon absorption difference scattering signal:

$$\frac{d\sigma}{d\Omega} \sim S_0(Q,t) + P_2(\cos\theta_Q)S_2(Q,t)$$

U. Lorenz, *et al.*, New J. Phys. **12**, 113022 (2010)
E. Biasin, et al., J. Synchrtron Rad. 25, 306 (2018)

Experiment performed at LCLS

Temporal evolution of an ensemble of randomly oriented PtPOP molecules before and after excitation



Scheme of the pump-probe experiment at LCLS

Angular X-ray Cross-Correlation Analysis

Cross-correlation functions:

$$\mathrm{C}(q,\Delta) = \left\langle I^{dif}(q,\varphi) I^{dif}(q,\varphi+\Delta) \right\rangle_{\varphi}$$

where:

$$I^{dif}(q,\varphi) = I^{on}(q,\varphi) - I^{off}(q,\varphi)$$

Angular Fourier series:

$$\mathrm{C}(q,\Delta) = \sum_{n=-\infty}^{\infty} C_n(q) e^{in\Delta}$$

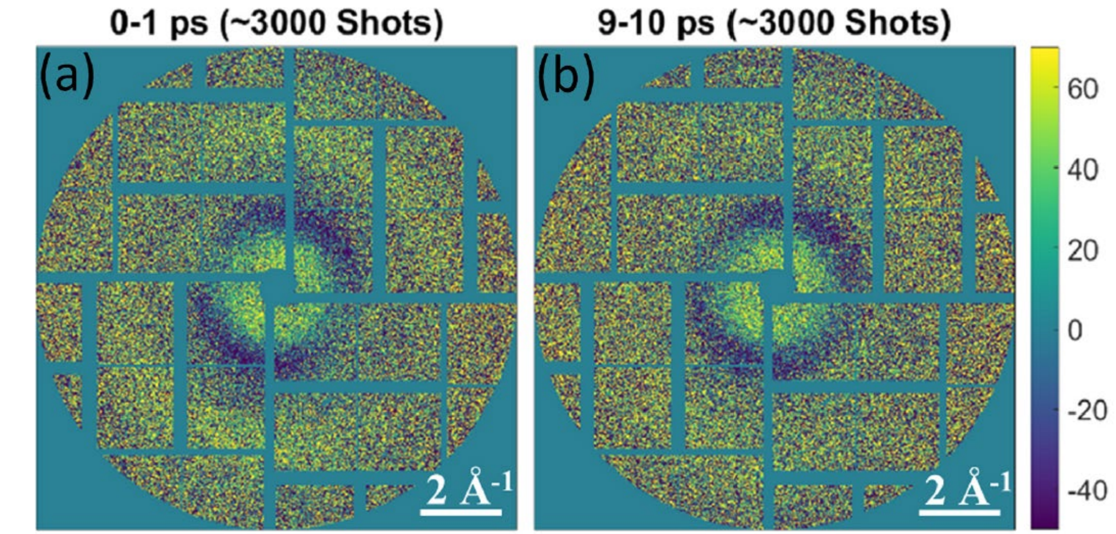
$$C_n(q) = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{C}(q,\Delta) e^{-in\Delta} d\Delta$$

And we know that:

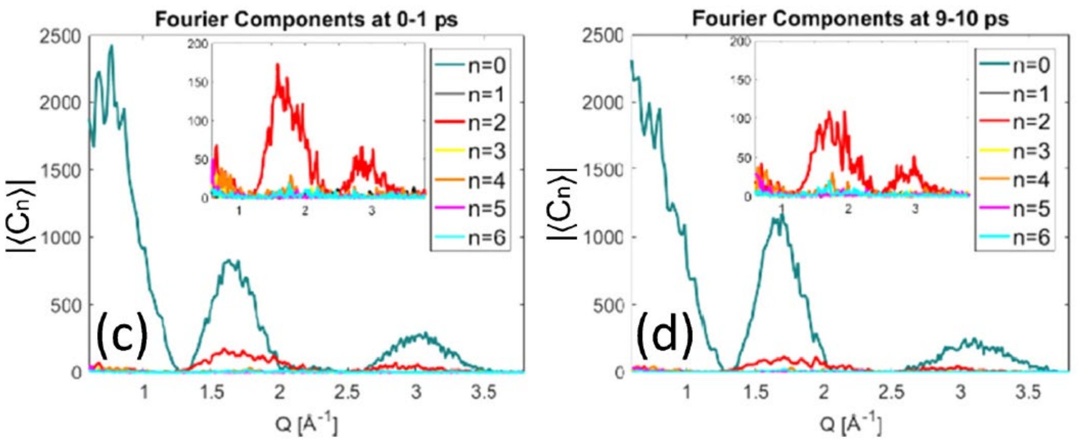
$$C_n(q) = \left| I_n^{dif}(q) \right|^2$$

Angular X-ray Cross-Correlation Analysis

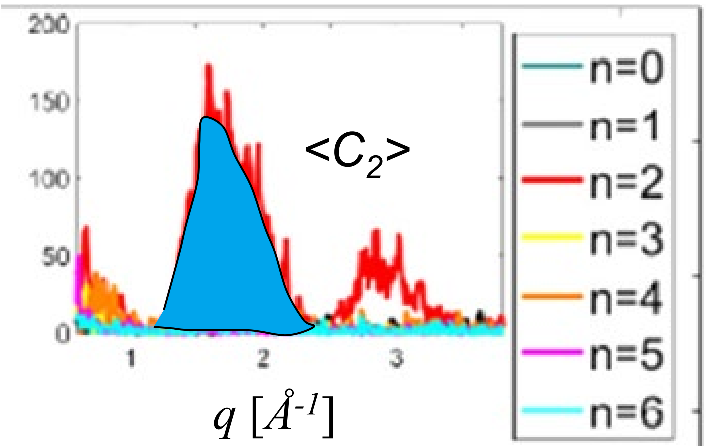
Difference scattering detector images $I^{dif}(\boldsymbol{q})$ for two different time delay intervals



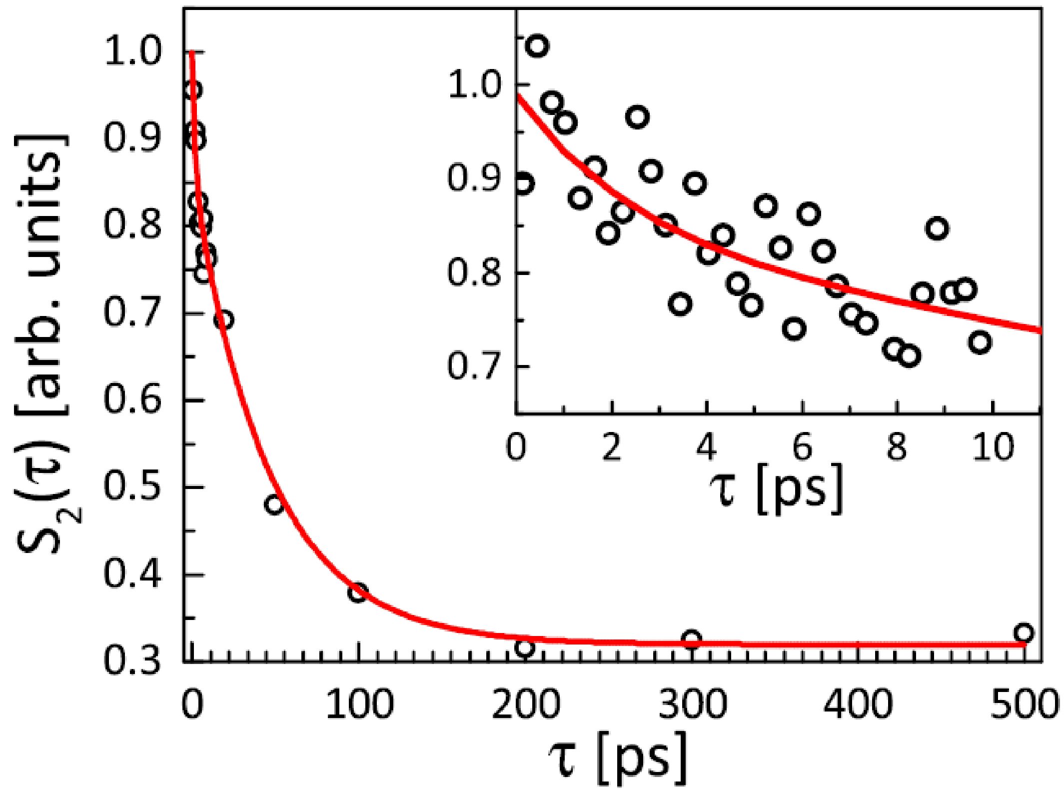
Calculated averaged FC's of the CCFs



Characteristic times



$$S_2(\tau) = \int \sqrt{\langle C_2(q,\tau)\rangle} dq$$



Double exponential fit

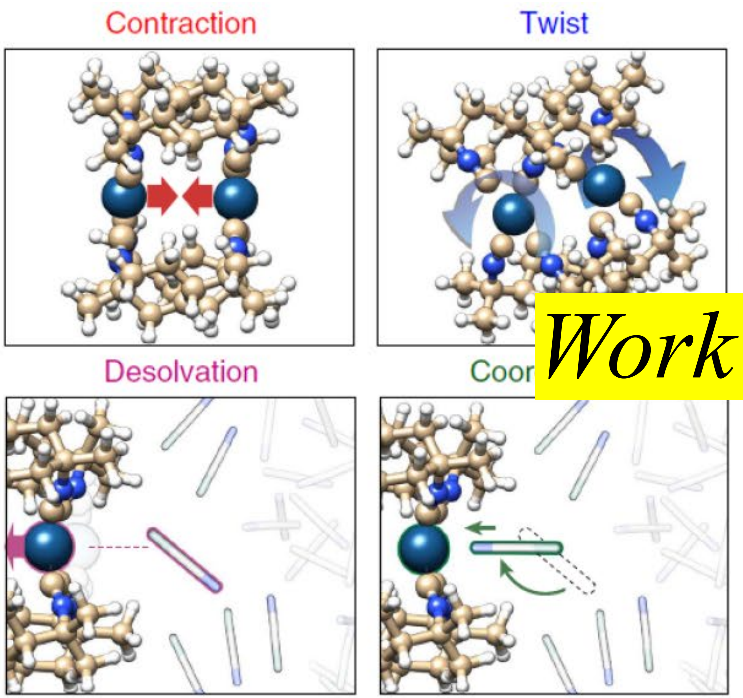
$$S_2(\tau) = Ae^{-t/\tau_1} + Be^{-t/\tau_2} + C$$

$$\tau_1 = 1.9 \pm 1.5\ ps$$

$$\tau_2 = 46 \pm 10\ ps$$

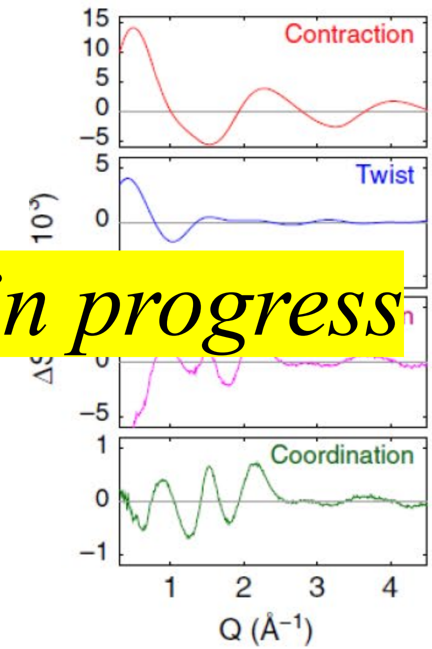
LCLS experiment (2018)

Ir_2(Dim)4 complexes

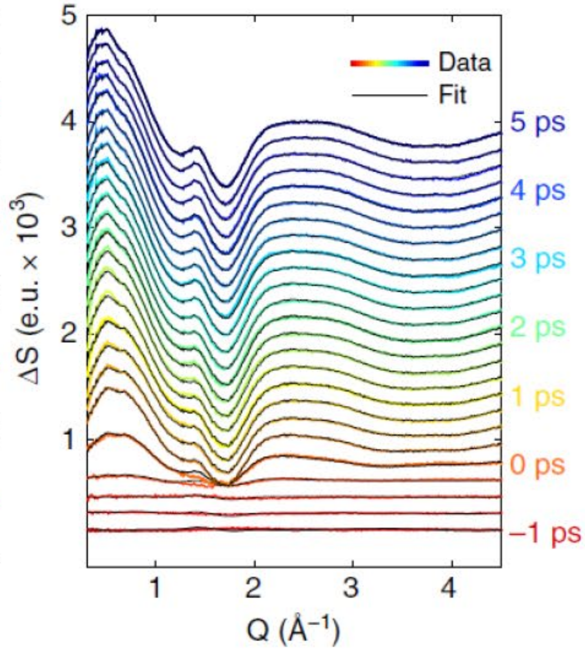


Possible dynamics in Ir_2(Dim)4

Work in progress



Difference scattering contribution



Difference scattering signal
LCLS Experiment (2012)

Summary

- AXCCA is a powerful tool to study ordered and partially ordered systems
- Can be applied to study details of correlations between long range bond-orientational order and short range positional order in liquid crystals
- Can be applied to study details of organization in mesocrystals formed by nanocrystals
- Can be applied to determine structure of molecular systems excited by laser pulses
- and much more…

Thank you for your attention