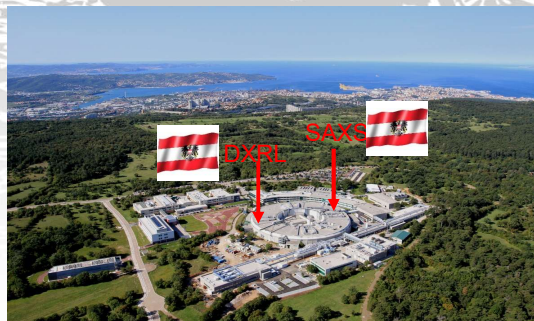


Small Angle Scattering SAX(-ray)S / SAN(eutron)S

Heinz Amenitsch
TU-Graz & Austrian SAXS beamline, ELETTRA



Elettra Sincrotrone Trieste

fAnorganische
CHEMIE

Layout

2

PART I: Introduction to SAS

- ☐ Introduction to the Theory ("Graz School")
- ☐ From Experiments to Real Space
- ☐ Bio-SAXS ("Hamburg School")

PART II: SAXS applications in life science and material science using synchrotron

- ☐ Examples:
 - Chemistry
 - Hierarchical Materials
- ☐ Grazing Incidence SAXS ("no school")
 - Biomembranes
 - *In situ* Chemistry
- ☐ Some Aspects of Current Research

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Soft Condensed Matter

(© P. Schurtenberger)

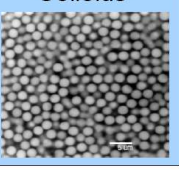


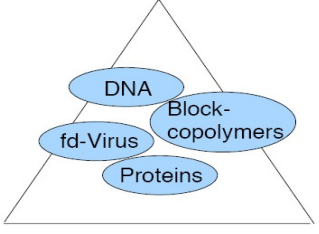
3

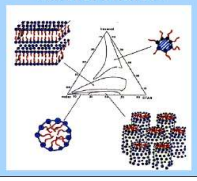
Soft Matter -
„complex fluids“
world between
fluid and solid

Polymers


Length- and
Timescales
Contrasts

Colloids




Surfactants


Equilibrium
and
Non-Equilibrium
States

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

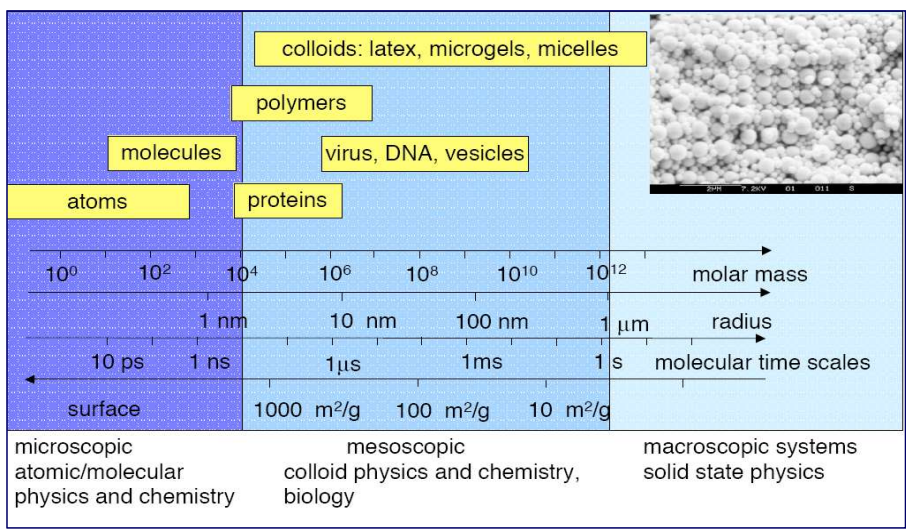


Characteristic length and time scales

(© P. Schurtenberger)



4



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Institute of Chemistry, University of Graz,
Austria

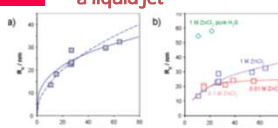
2



Research topics

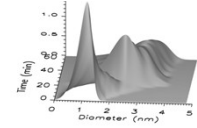
5

ZnS NPs growth in a liquid jet



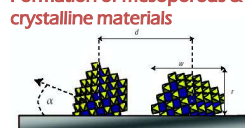
W. Schmidt, et al., JACS (2010), 132, 6822-6826

CdS nucleation and growth

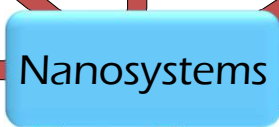


Viswanatha, R. et al. J. Phys. Chem. Lett. 1, 304 (2010)

Formation of mesoporous & crystalline materials



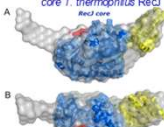
Grosso, D. et al. Nature Materials 2004, 3, 787-792.



Nanosystems

Proteins

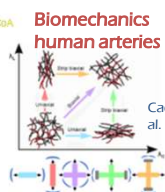
core T. thermophilus RecJ



helical domain of the acyl-CoA

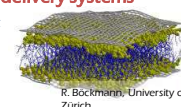
Krastanova I. et al. J. Biol. Chem. (2012)

Biomechanics human arteries



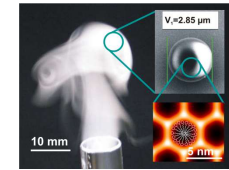
Cacho-Nerin, F., et al. (2015)

Biomembranes & drug delivery systems



Rappolt M, Pabst G, R. Bockmann, University of Zurich, P. Mariani et al.

Mesostructured SiO₂ produced by aerosol reaction



I. Shyjunon, et al., Rev. Scient. Instr., 79 (4), 043905 (2008), Langmuir (2011)

SILS School 2026

amenitsch@tugraz.at & amenitsch@elettra.trieste.it

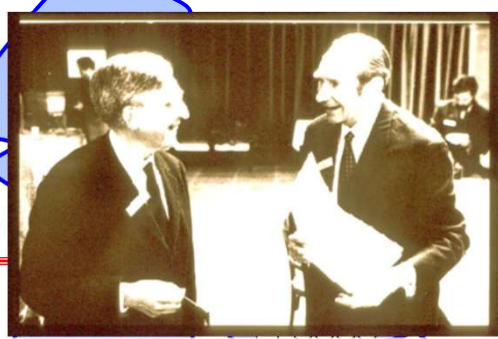
Anorganische CHEMIE





SAXS and WAXS

6



Andre Guinier **Otto Kratky**

The pioneers of Small Angle Scattering

DETECTOR

Beam Stop

SAXS

WAXS

X-rays



SILS School 2026

amenitsch@tugraz.at & amenitsch@elettra.trieste.it

Anorganische CHEMIE



7

SAXS and WAXS



Small – Angle : Supramolecular Envelope

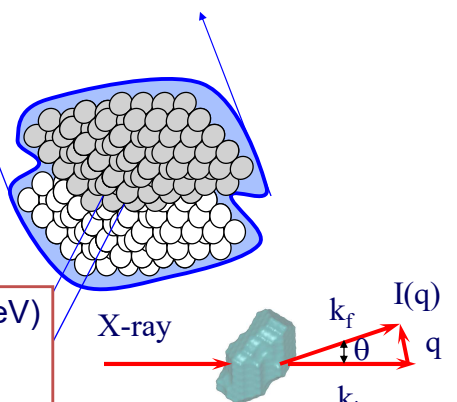
Bragg's law:

$$\sin \theta/2 = \lambda / 2d$$

small θ
large d

For CuK_α 0.154 nm (8 keV)

20 deg	0.5 nm
0.9 deg	10 nm
0.09 deg	100 nm



Molecular Lattice

SILS School 2026

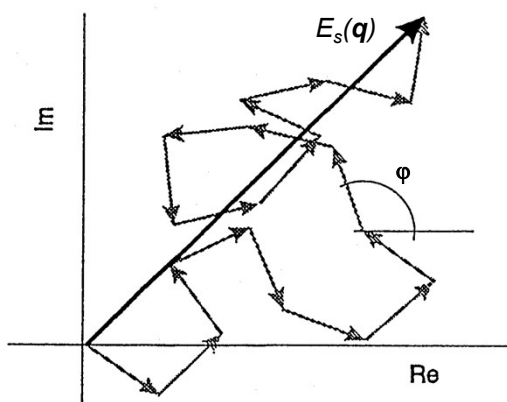
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it



8

The Scattered Field $E_s(q)$





The scattering amplitudes of all coherently scattered waves have to be added according to their amplitude and relative phase φ .

The phase difference depends on the relative location of the scattering centers.

SILS School 2026

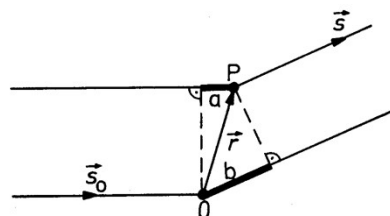
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it



The Phase Difference φ and the Scattering Vector $\mathbf{q}$



9



$$a = \vec{r} \cdot \vec{s}_0$$

$$b = \vec{r} \cdot \vec{s}$$

The path length difference is given by the length difference between the two paths a and b:

$$a - b = r\vec{s}_0 - r\vec{s} = -r(\vec{s} - \vec{s}_0)$$

The phase difference φ is given by the wave number ($2\pi/\lambda$) times the path length difference:

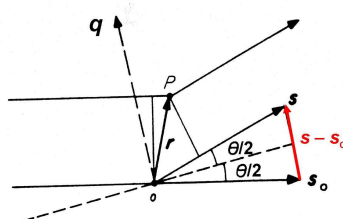
$$\varphi = -(2\pi/\lambda)r(\vec{s} - \vec{s}_0)$$

Now we introduce the scattering vector $\mathbf{q}$:

$$\mathbf{q} = (2\pi/\lambda)(\vec{s} - \vec{s}_0) \rightarrow \varphi = -\mathbf{q} \cdot \mathbf{r}$$

Its magnitude is:

$$q = 4\pi/\lambda \sin \theta/2$$



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



The Scattered Field $E_s(\mathbf{q})$



10

In order to find the total scattered field we have to integrate over the whole illuminated scattering volume V

$$E_s(\mathbf{q}) = \text{const} \int_V \rho(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r}$$

We can now express the density $\rho(\mathbf{r})$ by its mean $\bar{\rho}$ and its fluctuations $\Delta\rho(\mathbf{r})$:

$$\rho(\mathbf{r}) = \bar{\rho} + \Delta\rho(\mathbf{r})$$

The Fourier integral is linear, so we can rewrite the above equation:

$$E_s(\mathbf{q}) = \text{const} \left[\int_V \bar{\rho} \cdot e^{-i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r} + \int_V \Delta\rho(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r} \right]$$

Taking into account the large dimension of the scattering volume we get:

$$E_s(\mathbf{q}) = \text{const} \int_V \Delta\rho(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r}$$

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



From Scattering Amplitudes to Scattering Intensities

11

For monodisperse dilute systems we can write:

$$I_s(q) = N \langle |E_1(q)|^2 \rangle = N I_1(q)$$

We have introduced the single particle scattering amplitude $E_1(q)$ which is the scattered field resulting from integration over the particle volume only.

$$E_1(q) = \int_V \Delta\rho(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r}$$

$$|E_1(q)|^2 = E_1(q) \cdot E_1^*(q) = \int_V \int_V \Delta\rho(\mathbf{r}_1) \Delta\rho(\mathbf{r}_2) e^{-i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)} d\mathbf{r}_1 d\mathbf{r}_2$$

We put $\mathbf{r}_1 - \mathbf{r}_2 = \mathbf{r}$ and use $\mathbf{r}_2 = \mathbf{r}_1 - \mathbf{r}$ and introduce the *convolution square* of the density fluctuations:

$$\gamma(\mathbf{r}) \equiv \Delta\tilde{\rho}^2(\mathbf{r}) = \int_V \Delta\rho(\mathbf{r}_1) \Delta\rho(\mathbf{r}_1 - \mathbf{r}) d\mathbf{r}_1$$

SILS School 2026

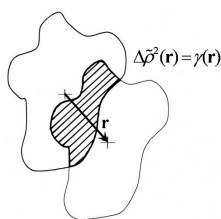
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

 **Anorganische
CHEMIE**

The Convolution Square of the Density Fluctuations

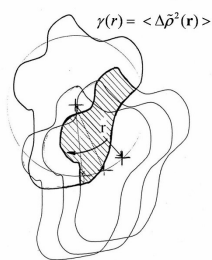
12

$\gamma(\mathbf{r})$ and $\gamma(r)$:



The function $\gamma(\mathbf{r})$ is calculated by shifting the “ghost” particle a vector $\mathbf{r}$ and integrating the overlapping volume.

This function is also called *spatial autocorrelation function (ACF)*.



The spatially averaged convolution square $\gamma(r)$ results from the same process, the ghost is shifted by a distance $r = |\mathbf{r}|$, but we have to average over all possible directions in space.

$$\gamma(r) = \tilde{\rho}^2(r) - V(\bar{\rho})^2 = \langle \Delta\tilde{\rho}^2(\mathbf{r}) \rangle = \left\langle \int_V \Delta\rho(\mathbf{r}_1) \Delta\rho(\mathbf{r}_1 - \mathbf{r}) d\mathbf{r}_1 \right\rangle$$

SILS School 2026

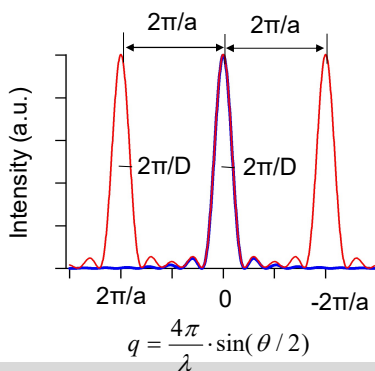
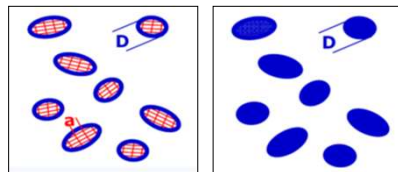
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

 **Anorganische
CHEMIE**

SAXS and WAXS



13



SAXS:

peak width (+ shape) → particle size

WAXS:

positions → lattice (type, spacings, strain)

width + shape → particle size

+ lattice strain fluctuations

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



RDG: Spatially Averaged Intensity $I(q)$



14

The spatially averaged intensity $I(q)$ is given by:

$$I(q) = \langle |E_1(\mathbf{q})|^2 \rangle = \langle \int_V \Delta \tilde{\rho}^2(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} d\mathbf{r} \rangle$$

$$= 4\pi \int_0^\infty \gamma(r) r^2 \frac{\sin qr}{qr} dr$$

by introducing the *pair distance distribution function* (PDDF) $p(r)$ with

$$p(r) = \gamma(r) \cdot r^2 = \Delta \tilde{\rho}^2(r) \cdot r^2$$

we finally get

$$I(q) = 4\pi \int_0^\infty p(r) \frac{\sin(qr)}{qr} dr$$

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

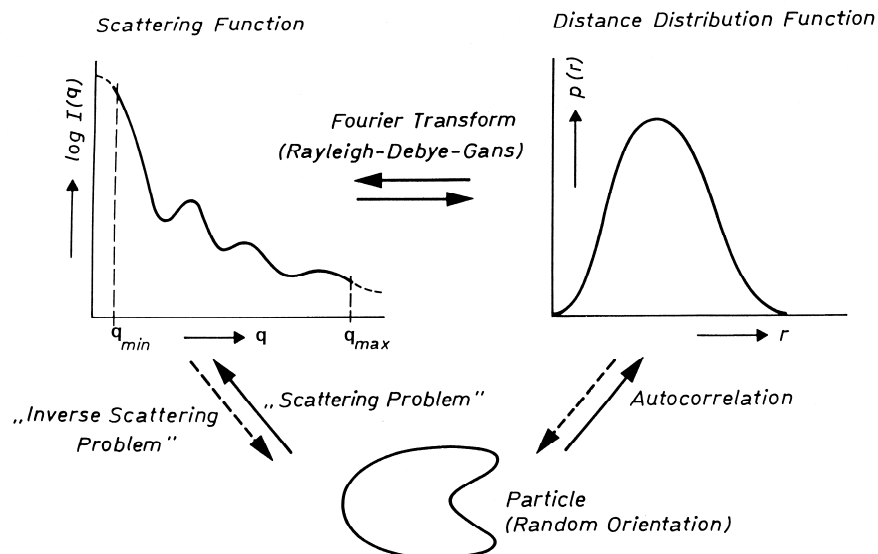
fAnorganische
CHEMIE



The Scattering Problem and the Inverse Scattering Problem



15



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

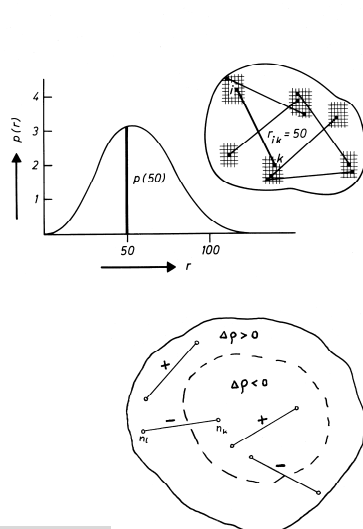
fAnorganische
CHEMIE



Definition of the Pair Distance Distribution Function (PDDF) $p(r)$



16



We can relate the meaning of a distance histogram to the PDDF $p(r)$ if the particles are homogeneous. The height of $p(r)$ is proportional to the number of distances that can be found inside the particle within the interval r and $r+dr$

The $p(r)$ function of inhomogeneous particles is proportional to the product of the difference scattering lengths $n_i n_k$ [$n_i = \Delta\rho(\mathbf{r}_i) dV(\mathbf{r}_i)$] of two volume elements i and k with a center-to-center distance between r and $r+dr$ and we sum over all pairs with this distance.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



RDG: The Particle Form Factor



17

$$I_s(q) = NI_1(q) = NI_1(0)P(q)$$

$I_1(0) = V^2 \Delta \rho^2$ intensity of single particle at $q = 0$

$P(q)$ particle form factor, where

$$P(q) = \frac{I_1(q)}{I_1(q \rightarrow 0)}$$

The normalized form factor $P(q)$ contains information about size and structure of the particle.

Form factor of a homogeneous sphere:

$$P(q) = \left[\frac{3(\sin qR - qR \cos qR)}{(qR)^3} \right]^2$$

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

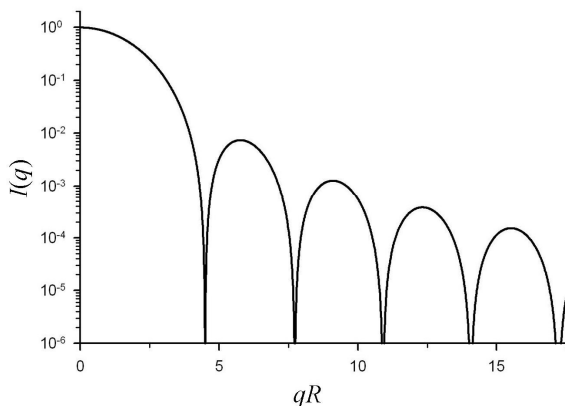
fAnorganische
CHEMIE



The Particle Form Factor



18



The function has minima for $\tan(qR) = qR$, or $qR = 4.49, 7.73, \dots$

SILS School 2026

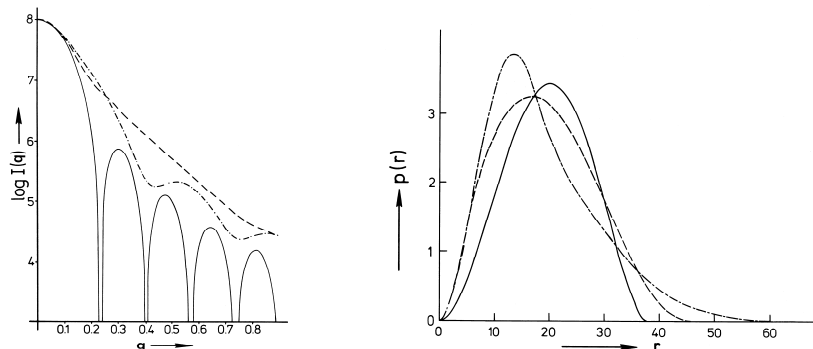
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Different Shapes of Homogeneous Particles

19



Comparison of a sphere (full line) an oblate ellipsoid (dashed line) and a prolate ellipsoid with the same volume.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Rod-like Particles

20

Let us regard a rod of length L and of cross-section A_c = The cross-section A_c (with maximum dimension d) should be small in comparison to the length of the whole particle L ($d \ll L$). For $q > 1/L$ we can write

$$I(q) = \frac{L\pi}{q} \cdot I_c(q)$$

The cross-section scattering function $I_c(q)$ is related to the cross-section distance distribution $p_c(r)$ by

$$I_c(q) = 2\pi \int_0^\infty p_c(r) J_0(qr) dr$$

where

$$p_c(r) = \gamma_c(r) \cdot r = 2\pi r \int_{A_c} \Delta\rho_c(r') \Delta\rho_c(r' + r) dr$$

SILS School 2026

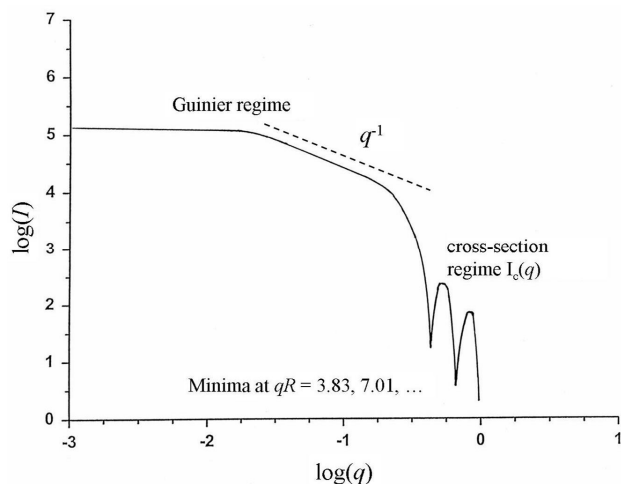
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Scattering Function for a Long, Rod-like Particle Schematic Representation



21



The different regimes can be visualized in a $\log(I)$ vs. $\log(q)$ plot of the scattering curve:

The Guinier regime, the q^{-1} regime and the cross-section regime.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

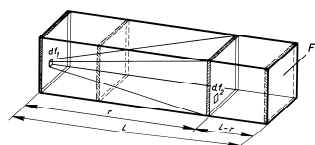
fAnorganische
CHEMIE



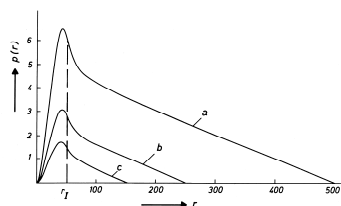
PDDF's for Rod-like Particles



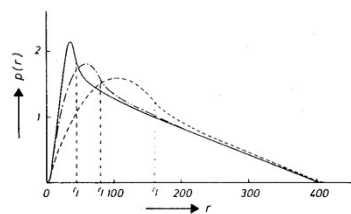
22



$$p(r) = \frac{2}{4\pi} \int_r^L \int_A \int_A \Delta \rho^2 df_1 df_2 dx = \frac{I}{2\pi} \Delta \rho^2 A_c^2 (L - r),$$



PDDF from homogeneous prisms with edge lengths of: (a) 50:50:500, (b) 50:50:250 and (c) 50:50:150



PDDF for three parallel epipeds with constant length L (400 Å) and constant cross-section area A_c but varying length of the edges: 40:40, 80:20 and 160:10.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Flat Particles

23

Let us now consider a flat particle, with a finite and constant thickness D_t , being extremely large in the two other dimensions with an area A . In full analogy to the case of the rod we can separate the scattering amplitude into a *planar factor* $2\pi Aq^{-2}$ and a *thickness-factor* $I_t(q)$, i.e. the total intensity is given by

$$I(q) = I_{\text{plane}} \cdot I_t(q) = \frac{2\pi A}{q^2} \cdot I_t(q).$$

The thickness-factor is related to the thickness distance distribution $p_t(r)$ by

$$I_t(q) = 2 \int_0^\infty p_t(r) \cos(qr) dr$$

where

$$p_t(r) = \gamma_t(r) = 2 \int_0^\infty \Delta\rho_t(r') \Delta\rho(r' + r) dr.$$

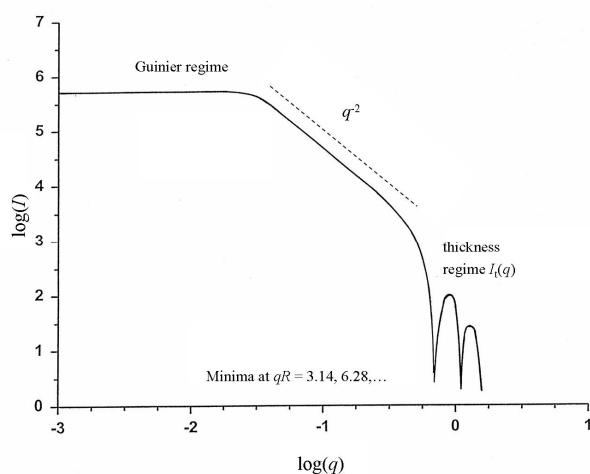
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Scattering Function for a Flat, Lamellar Particle. Schematic Representation

24



The different regimes can be visualized in a $\log(I)$ vs. $\log(q)$ plot of the scattering curve:

The Guinier regime, the q^{-2} regime and the thickness regime.

SILS School 2026

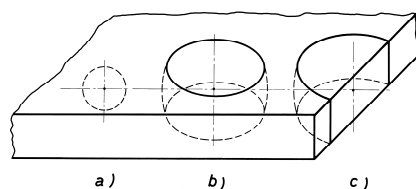
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

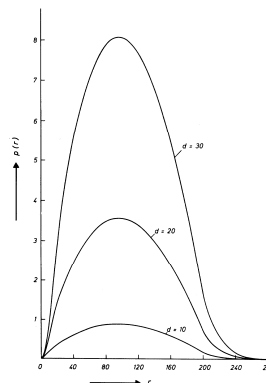
PDDF's for Flat Particles



25



Sketch for the qualitative discussion of the PDDF of a flat particle



PDDFs of lamellar particles with the same basal plane ($200 \times 200 \text{ Å}$) and different thickness D_t : (a) $D_t = 10 \text{ Å}$, (b) $D_t = 20 \text{ Å}$ and (c) $D_t = 30 \text{ Å}$.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

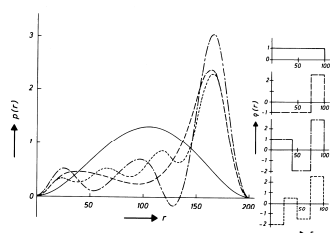


Inhomogeneous Particles:

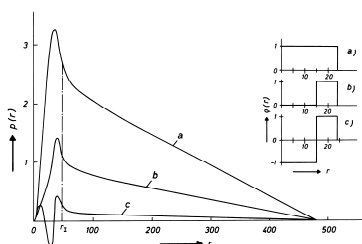


26

Spheres and Cylinders with Radial Inhomogeneity



Spherical multilayer models with constant outer diameter of 200 Å . PDDFs in the left part, density profiles in the right part of the figure.



Circular cylinders with a constant length of 480 Å and an outer diameter D_c of 48 Å . (a) Homogeneous cylinder, (b) hollow cylinder, (c) inhomogeneous cylinder. The PDDFs are shown on the left, the corresponding radial density distributions $\rho(r)$ on the right.

SILS School 2026

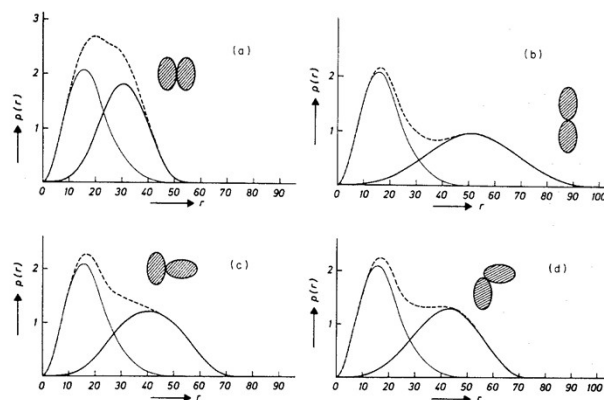
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Aggregates - Dimers

27



PDDFs from dimer models built from prolate ellipsoids. Monomers (full line), dimers (broken line), and difference between dimers and monomers (thick full line).

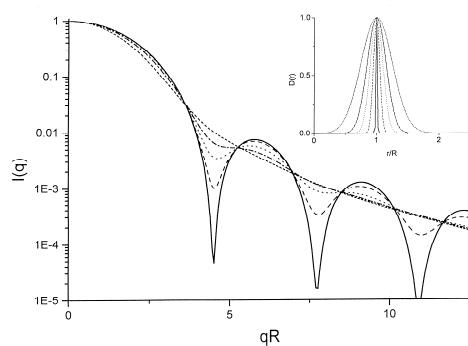
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Polydisperse Systems

28



Intensity Distribution

$$I(q) = c_i \int_0^{\infty} D_i(R) \cdot P_0(q, R) dR$$

Volume or Mass Distribution

$$I(q) = c_v \int_0^{\infty} D_v(R) \cdot R^3 \cdot P_0(q, R) dR$$

Number Distribution

$$I(q) = c_n \int_0^{\infty} D_n(R) \cdot R^6 \cdot P_0(q, R) dR$$

Scattering curves of Gaussian size distributions of spheres with varying width (see inset).

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Radius of Gyration



29

The radius of gyration is one of the most important parameters in the field of small-angle scattering. In full analogy to the radius of inertia in mechanics it is defined as

$$R_g^2 = \frac{\int \Delta\rho(r_i) r_i^2 dV_i}{\int \Delta\rho(r_i) dV_i}$$

According to the momentum theorem of Fourier transformation the second moment of a function in one space is related to the second derivative (curvature) of its Fourier transform at the origin. This relation is the basis of the so-called *Guinier approximation* for the description of $I(q)$ for low q derived from a series expansion:

$$I(q) = I(0) e^{-\frac{q^2 R_g^2}{3}}$$

We can also use another relation for the estimation of the radius of gyration:

$$R_g^2 = \frac{\int p(r) r^2 dr}{2 \int p(r) dr}$$

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



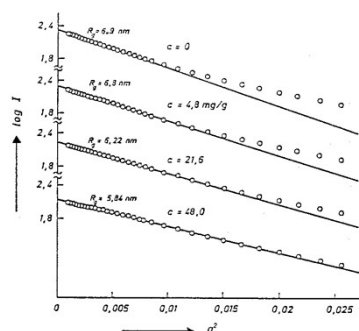
Radius of Gyration - Guinier Plot



30

From the previous equation it is clear that we can calculate the radius of gyration from the PDDF once it is known. Otherwise we can use the Guinier approximation to determine R_g directly from the scattering data with a so-called *Guinier-plot*.

Plotting $\ln(I(q))$ vs q^2 we get a straight line with a slope proportional to R_g^2 .



Example for a Guinier plot from scattering data of a protein solution with varying concentration, including an extrapolation to zero concentration.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Radius of Gyration of the Cross-Section



31

For rod-like particles we can also define a radius of gyration of the cross-section which can be calculated from $p_c(r)$ by

$$R_c^2 = \frac{\int p_c(r) r^2 dr}{2 \int p_c(r) dr}$$

or it can be estimated in reciprocal space form

$$I_c(q) = I_c(0) e^{-\frac{q^2 R_c^2}{2}}$$

by a so-called cross section Guinier plot $[\log(I(q)q) \text{ vs. } q^2]$.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Radius of Gyration of the Thickness Function



32

For lamellar particles we can also define a radius of gyration of the thickness function which can be calculated from $p_t(r)$ by

$$R_t^2 = \frac{\int p_t(r) r^2 dr}{2 \int p_t(r) dr}$$

or it can be estimated in reciprocal space form

$$I_t(q) = I_t(0) e^{-q^2 R_t^2}$$

by a so-called thickness Guinier plot $[\log(I(q)q^2) \text{ vs. } q^2]$.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

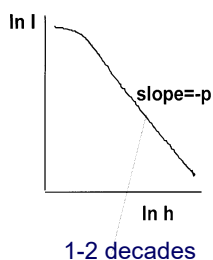


Porod Limit - Porod Plot - Fractals

33

We proceed now to the discussion of the **final slope** of the scattering curve at high q -values, we may expect this to depend mainly on the fine structure of the particle.

$$I(q)_{q \rightarrow \infty} = (\Delta\rho)^2 \cdot \frac{2\pi}{q^4} \cdot S$$



For mass fractals, where
 $1 < D < 3$, and $M \propto R^D$
 it holds, that
 $p = D$

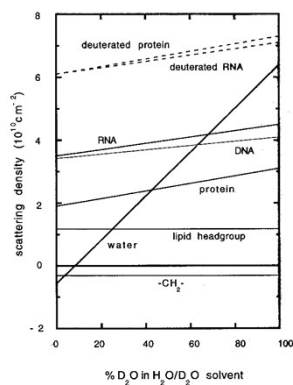
For surface fractals, where
 $2 < D_s < 3$
 it holds, that
 $p = 6 - D_s$

SILS Sch

organische
CHEMIE

Contrast Variation: Index Match

34



A mixture of H₂O and D₂O allows to match different regions in a sample.



When the monster came, Lola, like the peppered moth and the arctic hare, remained motionless and undetected, Harold, of course, was immediately devoured!

Autrans '94 R. May (found in „Los Alamos Science“)

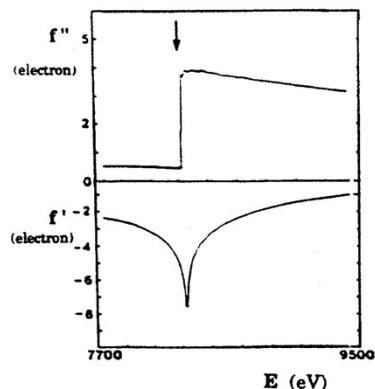
SILS School 2026

amenitsch@tugraz.at &
 amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Contrast Variation in SAXS by Anomalous Scattering

35



Typical energy dependence of f' and f'' near the absorption edge of an element. Shown here is the nickel K edge at 8333 eV.

This method, also known as *resonant small angle scattering* uses another possibility for the variation of the contrast. Near the inner shell absorption edge, the coherent scattering length or atomic scattering factor of an atom is a function of the energy E of the X-ray photon:

$$f(E) = Z + f'(E) + if''$$

Energy variation is only possible with the "white" X-ray beam of a synchrotron. The main problem for applications in chemistry is the fact that the edges for C, H, N and O are outside the useful energy window at very low energies. In solution experiments this effect might be useful for heavy counter ions (Br^+) in micellar systems.

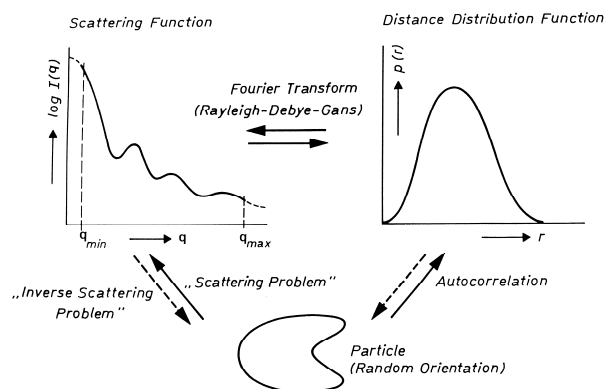
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

The Scattering Problem and the Inverse Scattering Problem

36



For the solution of the inverse Problem it is essential to be able to calculate the PDDF from the experimental scattering curve with minimum termination effect.

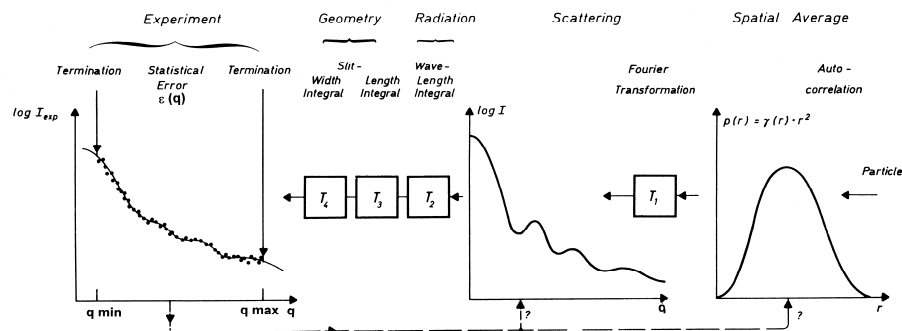
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

From experimental data to the PDDF

37



All Transformations T1 to T4 are linear and are mathematically well defined, this does not hold for their inverse transformations.

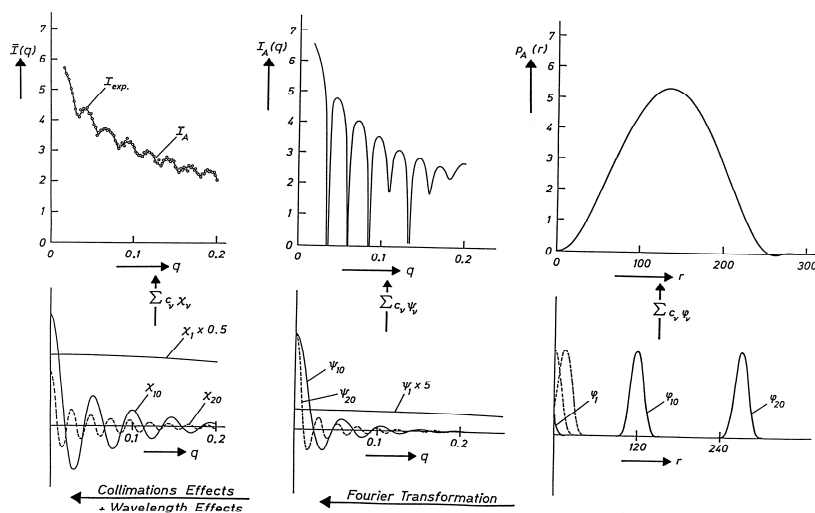
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

The Principles of the Indirect Fourier Transformation

38



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Other IFT Applications - Equations



39

Summary of the different transforms T_1 used in *IFT*:

Arbitrary shape:

$$I(q) = 4\pi \int_0^\infty p(r) \frac{\sin(qr)}{qr} dr$$

Cylindrical Symmetry:

$$I(q) = \frac{2\pi^2 L}{q} \int_0^\infty p_c(r) J_0(qr) dr$$

Lamellar Symmetry:

$$I_{plane}(q) = \frac{4\pi A}{q^2} \int_0^\infty p_l(r) \cos(qr) dr$$

The structure is the same for all equations, just the kernels of the integrals differ!

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

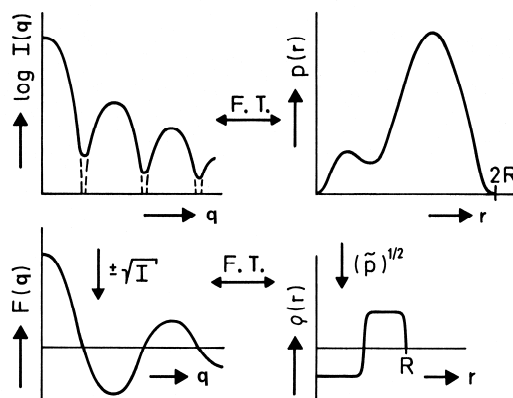
fAnorganische
CHEMIE



Deconvolution of the PDDF – The *Magic Square*



40



The *Magic square* of small-angle scattering: The correlations between the radial density $\Delta\rho(r)$ and the PDDF $p(r)$ and their Fourier transforms, the scattering amplitude $F(q)$ and scattering intensity $I(q)$ under the assumption of spherical symmetry.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Deconvolution of the PDDF – Principles I



41

Here we are facing a similar situation as in the *IFT* method: for a given density distribution $\rho(r)$ we can calculate the exact $p(r)$ -function for all three cases (spherical, cylindrical and lamellar symmetry) by a convolution square operation but we do not have a useful description of the inverse problem, the so-called convolution square root.

As an additional problem we have to keep in mind the fact, that the convolution square operation is a **nonlinear transformation** which will not allow an inversion by the solution of a simple linear least squares technique like in the case of the indirect Fourier transformation.

We start again with a series expansion of the radial density function $\rho(r)$ in the usual way:

$$\bar{\rho}(r) = \sum_{i=1}^N c_i \varphi_i(r)$$

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Deconvolution of the PDDF – Principles II



42

The approximation for the density profile corresponds to an approximation to the PDDF:

$$\bar{p}(r) = \sum_{i=1}^N V_{ii}(r) c_i^2 + 2 \sum_{i>k} V_{ik}(r) c_i c_k$$

The overlap integrals $V_{ik}(r)$ describe the overlapping of the *i*-th with the *k*-th step or shell where one function has been shifted an arbitrary distance *r*. These overlap or convolution integrals are very simple for the planar case (one-dimensional convolution of two step function leads simply to a triangle) but are a bit more complicated for the cylindrical and spherical case:

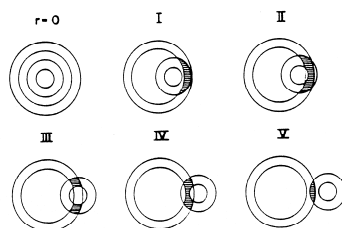


Illustration of the five sub-regions for the calculation of the overlap integrals $V_{ik}(r)$.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Deconvolution of the PDDF – Iterative Solution



43

The above equation for the PDDF is nonlinear in its coefficients c_i . The corresponding least squares problem has to be linearized by a series expansion where higher order terms are omitted.

Such linearized systems must be solved iteratively. In addition one needs starting values $c_i^{(0)}$ for the first iteration. Here we set all coefficients equal to a constant.

We then calculate the difference function

$$\Delta p(r) = p(r) - \bar{p}^{(0)}(r)$$

which would be zero only if we would know the exact coefficients c_i .

Now we calculate correction terms Δc_i in order to minimize $\Delta p(r)$ in a least square sense.

$$\sum_{i=1}^N V_{ii}(r) [(c_i + \Delta c_i)^2] + 2 \sum_{i>k} V_{ik}(r) [(c_i + \Delta c_i)(c_k + \Delta c_k) - c_i c_k] = \Delta p(r)$$

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it



Deconvolution of the PDDF – Iterative Solution II



44

We linearize this equation by omitting the second order terms Δc_i^2 and $\Delta c_i \Delta c_k$ and we get

$$2 \sum_{k=1}^N \sum_{i=1}^N c_i V_{ik}(r_j) \Delta c_k = \Delta p(r_j)$$

for $j = 1, 2, 3, \dots, M$ and $M > N$. These equations can be written in matrix notation

$$A_{jk} \Delta c_k = \Delta p_j \quad \text{or} \quad \mathbf{A} \Delta \mathbf{c}^{(0)} = \Delta \mathbf{p}^{(0)}$$

where the matrix elements A_{jk} are given by

$$A_{jk} = 2 \sum_{i=1}^N c_i V_{ik}(r_j)$$

This system is solved with a weighted least squares condition considering the standard deviations of the function $\Delta p(r)$ and we get the correction terms Δc .

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it



Deconvolution of the PDDF – Iterative Solution III



45

They allow the calculation of improved coefficients $c_i^{(1)}$:

$$c_i^{(1)} = c_i^{(0)} + \Delta c_i$$

and with these coefficients we start the next iteration, get further improvements and if this iterative procedure converges we have solved the problem.

This problem is, however, again an *ill-posed problem* so that we have to add again a stabilization criterion and we have to solve the nonlinear problem by iteration for every *Lagrange multiplier*.

Many applications performed in the meantime have shown that the deconvolution technique works well in combination with the indirect transformation method, also in cases where the conditions of symmetry are not perfectly fulfilled.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

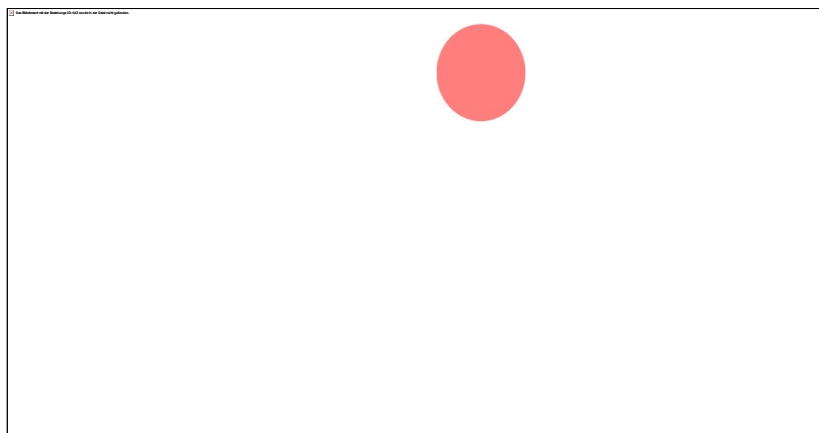
fAnorganische
CHEMIE



Surfactant Systems - Spherical micelles



46



Scattering pattern of spherical aggregates with radius R . The scattering curve $I(q)$ is the Fourier transform of the PDDF $p(r)$. This PDDF is the convolution square of the radial density distribution $\Delta\rho(r)$.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



SAXS 2.0: Theoretical Background



47

Assumption of monodisperse globular particles:

$$I(q) = n \cdot P(q) \cdot S(q)$$

n ... Particle density

q ... Scattering vector

$I(q)$... Scattering Intensity

$P(q)$... Form Factor $P(q) \leftrightarrow p(r)$

$S(q)$... Structure Factor $[S(q) - 1] \leftrightarrow [g(r) - 1]$

Interaction Potential: Hard Spheres Potential

Closure relation: Percus-Yevick-Approximation (analyt. Solution)

Kinning & Thomas, *Macromolecules* (1984), 17

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Fourier Transformation



48

$$I(q) = n \cdot P(q) \cdot S(q)$$

Form Factor $P(q) \leftrightarrow$ Pair Distance Distribution Function $p(r)$

$$P(q) = 4\pi \int_0^\infty p(r) \frac{\sin(qr)}{qr} dr$$

Structure Factor $[S(q) - 1] \leftrightarrow$ Total Correlation Function $[g(r) - 1] r^2$

$$S(q) - 1 = 4\pi n \int_0^\infty [g(r) - 1] r^2 \frac{\sin(qr)}{qr} dr$$

Due to the nearly identical structure of these equations it is obvious that it is not a trivial task to split the scattering intensity into these factors by mathematical means

GIFT (=General Indirect Fourier Transformation)

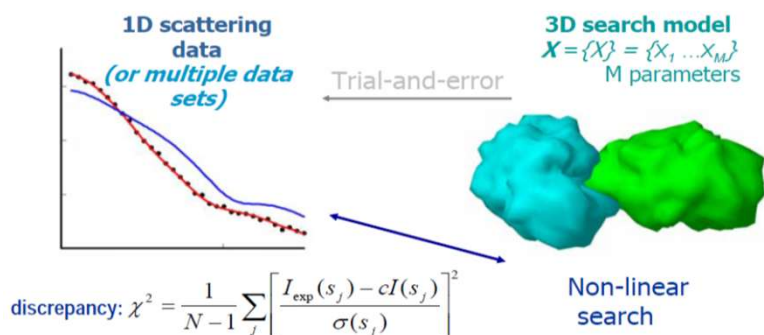
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

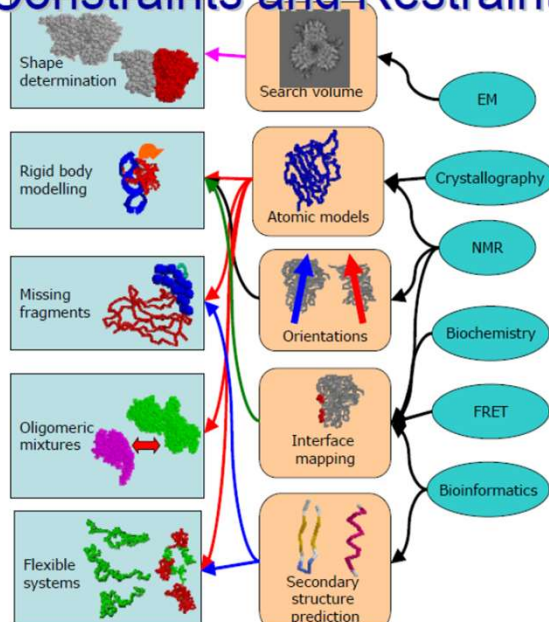


General principle of SAS modelling



Additional information is ALWAYS required to resolve or reduce ambiguity of interpretation at given resolution

Constraints and Restraints



Target function

- To reduce the ambiguity of data analysis

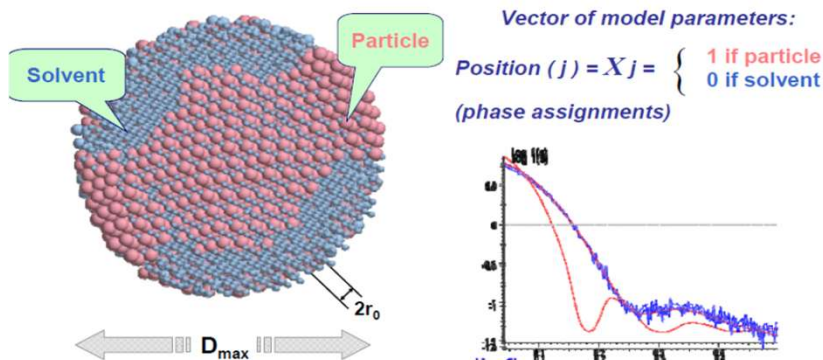
$$E(\{X\}) = \chi^2[(I(s), I_{\text{exp}}(s)] + \sum_i \alpha_i P_i$$

is minimized

- Penalties describe model-based restraints and/or introduce the available additional information from other methods: MX, NMR, EM etc)
- If the number of free parameters is small, a brute force (grid) search may be applied, otherwise a Monte-Carlo based technique (e.g. simulated annealing) is employed to perform the minimization of $E(\{X\})$

Ab initio shape determination

A sphere of radius D_{max} is filled by densely packed beads of radius $r_0 \ll D_{\text{max}}$



Svergun, D.I. (1999) *Biophys. J.* 76, 2879-2886

Bead Modelling: DAMMIN

- Scattering intensity is computed using spherical harmonics

$$A_{lm}^{(k)}(s) = i^l \sqrt{2/\pi} f(s) \sum_{j=1}^{N_k} j_l(sr_j) Y_{lm}^*(\omega_j)$$

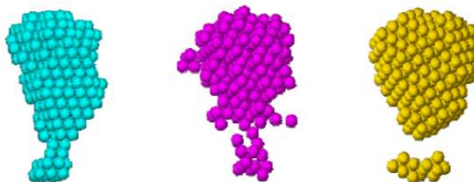
$$I(s) = 2\pi^2 \sum_{l=0}^{\infty} \sum_{m=-l}^l \left\{ \sum_{k=1}^K \left[\Delta\rho_k A_{lm}^{(k)}(s) \right]^2 + 2 \sum_{n>k} \Delta\rho_k A_{lm}^{(k)}(s) \Delta\rho_n \left[A_{lm}^{(n)}(s) \right]^* \right\}$$

- Penalty terms ensure compactness and connectivity

compact

loose

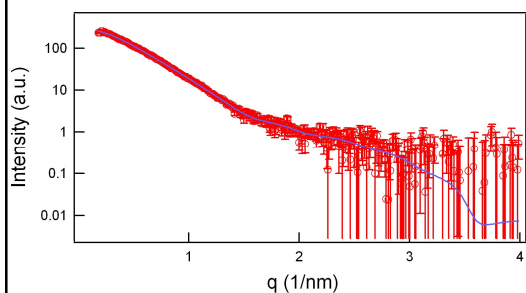
disconnected



Svergun, D.I. (1999) *Biophys. J.* 76, 2879-2886

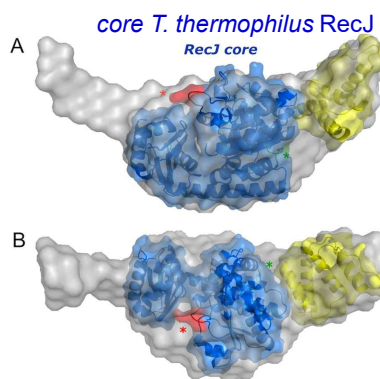
Scattering on human CDC45 Protein

CDC45 protein conserved in all eukaryotes
 initiation of DNA replication
 progression of the replication fork

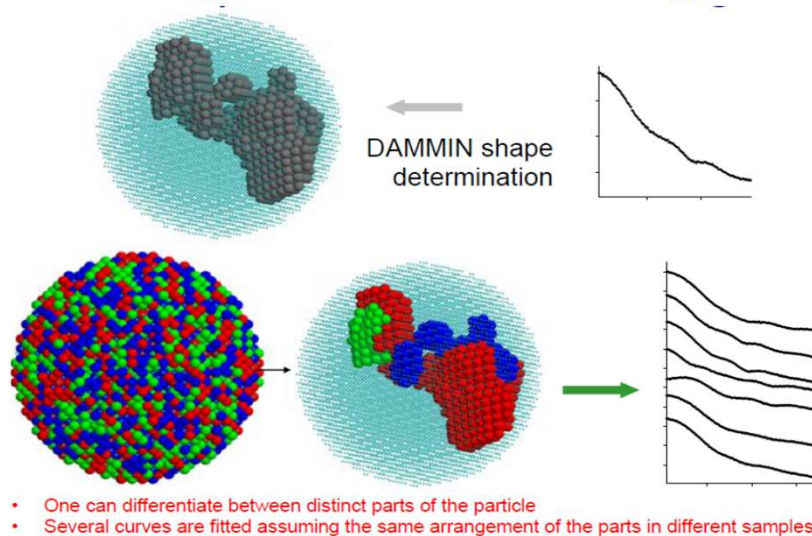


hCDC45, 1.85 mg/ml, 40μl, 30 s

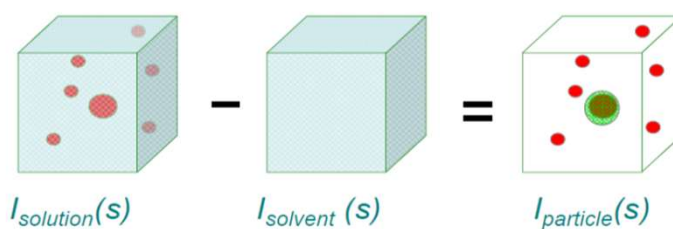
Kastranova I, Onesti S et al., *J.Biol.Chem.* (2012)



Multiphase bead modelling



How to compute SAS from atomic model



- ♦ To obtain scattering from the particles, solvent scattering must be subtracted to yield effective density distribution $\Delta\rho = \langle \rho(r) - \rho_s \rangle$, where ρ_s is the scattering density of the solvent
- ♦ Further, the bound solvent density may differ from that of the bulk

57

Scattering from a macromolecule in solution

TU Graz

Atomic scattering
 - Excluded volume
 + Shell scattering
 Envelope function $F(\omega)$

Internal cavities

SILS School 2026

amenitsch@tugraz.at &
 amenitsch@elettra.trieste.it

fAnorganische
 CHEMIE

58

Scattering from a macromolecule in solution

TU Graz

$$I(s) = \langle |A(s)|^2 \rangle_\Omega = \langle |A_a(s) - \rho_s E(s) + \delta \rho_b B(s)|^2 \rangle_\Omega$$

- ♦ $A_a(s)$: atomic scattering in vacuum (total scattering length / number of e^-)
- ♦ $E(s)$: scattering from the excluded volume (normalized)
- ♦ $B(s)$: scattering from the hydration shell (normalized)

CRY SOL (X-rays): Svergun et al. (1995). *J. Appl. Cryst.* **28**, 768
CRY SON (neutrons): Svergun et al. (1998) *P.N.A.S. USA*, **95**, 2267

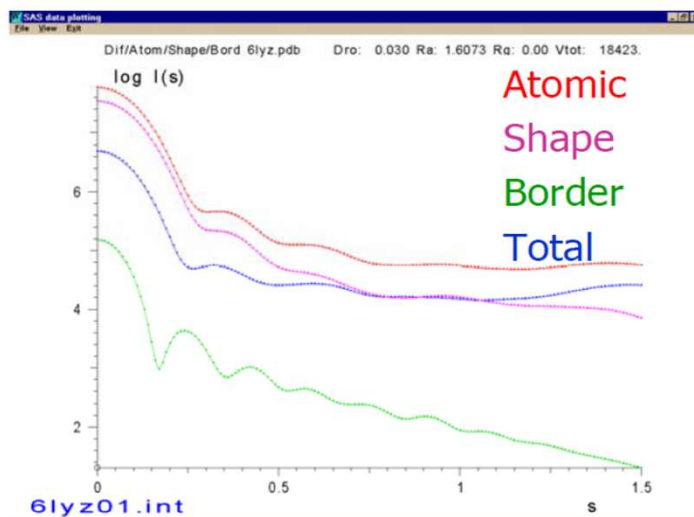
SILS School 2026

amenitsch@tugraz.at &
 amenitsch@elettra.trieste.it

fAnorganische
 CHEMIE

59

Scattering components (lysozyme)



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

f Anorganische
CHEMIE

60



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

f Anorganische
CHEMIE

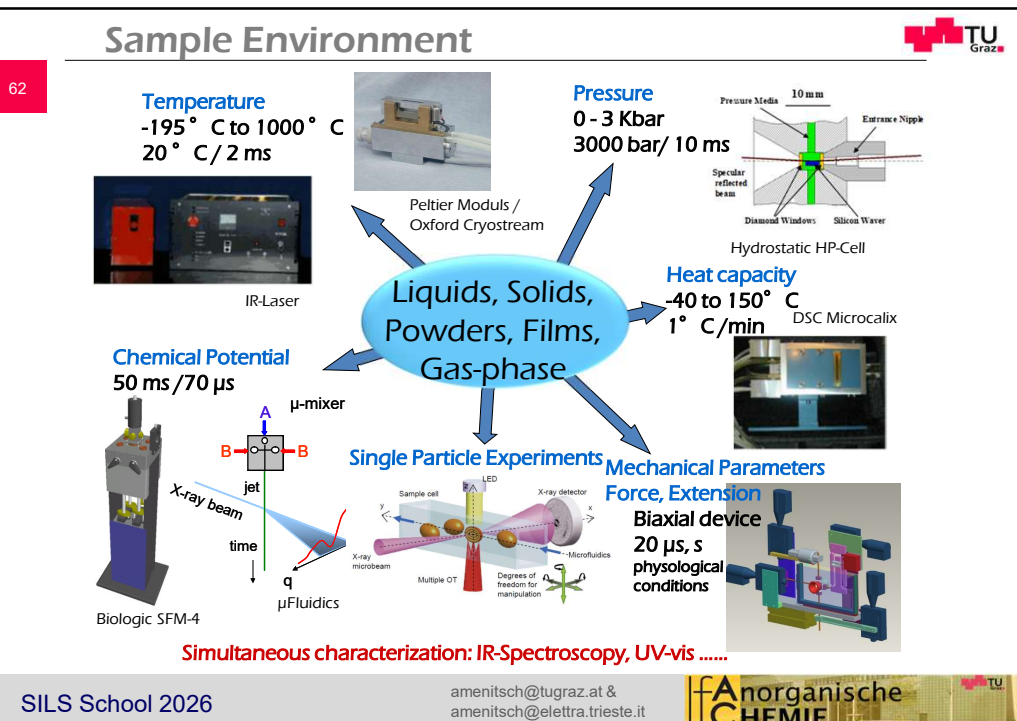
SAXS applications in life science and material science using synchrotron

Heinz Amenitsch
TU-Graz & Austrian SAXS beamline, ELETTRA



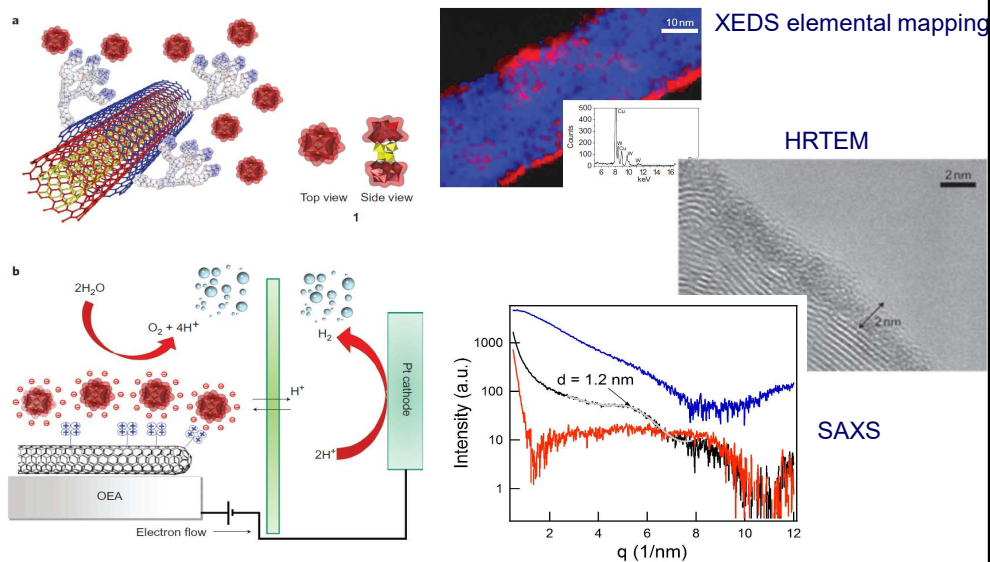
Elettra Sincrotrone Trieste

f Anorganische
CHEMIE



63

F.Toma, et al., Nature Chemistry, (2010), 10.1038/NCHEM.761

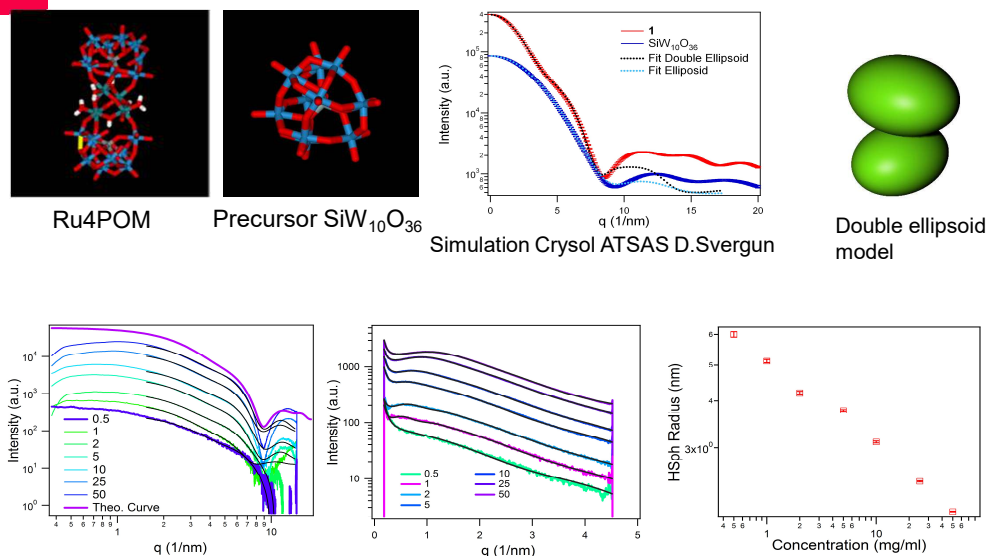


SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE

64

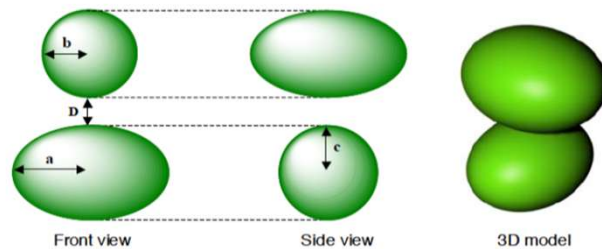


SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE

65



$$I_{\text{scat}} = I_0 \cdot \frac{1}{\pi} \int_0^\pi d\beta \int_0^{\pi/2} d\alpha \cdot \sin(\alpha) \cdot \frac{1}{4} \cdot F_{2\text{ellip}}(q, a, b, c, D, \alpha, \beta)^2 \quad (1)$$

$$F_{2\text{ellip}}(q, a, b, c, R, \alpha, \beta)^2 = (F_{\text{ellip}}(R_1, q) + F_{\text{ellip}}(R_2, q))^2 \cdot \cos(q \cdot (D/2 + c) \cdot \cos(\alpha))^2 + \\ + (F_{\text{ellip}}(R_1, q) - F_{\text{ellip}}(R_2, q))^2 \cdot \sin(q \cdot (D/2 + c) \cdot \cos(\alpha))^2$$

$$F_{\text{ellip}}(R, q) = 3 \cdot \frac{\sin(q \cdot R) - q \cdot R \cdot \cos(q \cdot R)}{(q \cdot R)^3}$$

$$R_1 = \sqrt{(a^2 \cdot \sin(\beta)^2 + b^2 \cdot \cos(\beta)^2) \cdot \sin(\alpha)^2 + c^2 \cdot \cos(\alpha)^2}$$

$$R_2 = \sqrt{(b^2 \cdot \sin(\beta)^2 + a^2 \cdot \cos(\beta)^2) \cdot \sin(\alpha)^2 + c^2 \cdot \cos(\alpha)^2}$$

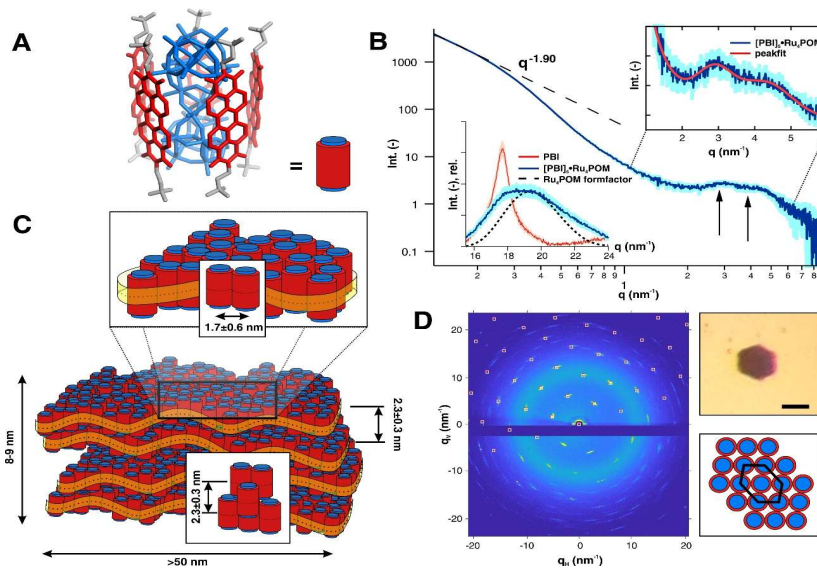
SILS School 2026

 amenitsch@tugraz.at &
 amenitsch@elettra.trieste.it

 fAnorganische
 CHEMIE

66

Artificial Quantasomes for Photo-assisted Water Oxidation



SILS School 2026

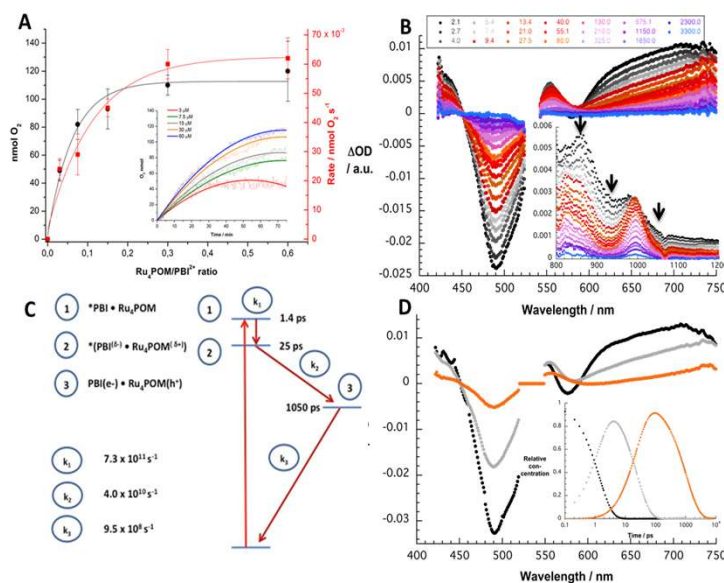
 amenitsch@tugraz.at &
 amenitsch@elettra.trieste.it

 fAnorganische
 CHEMIE

Artificial Quantasomes for Photo-assisted Water Oxidation



67



Marcella Bonchio,
Zois Syrgiannis,
Maurizio Prato et al.
Nature Chemistry
(2019)

SILS School 2026

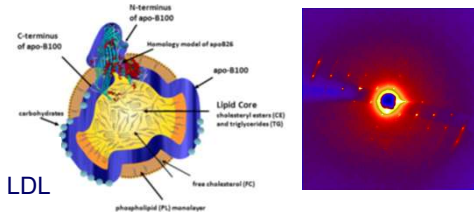
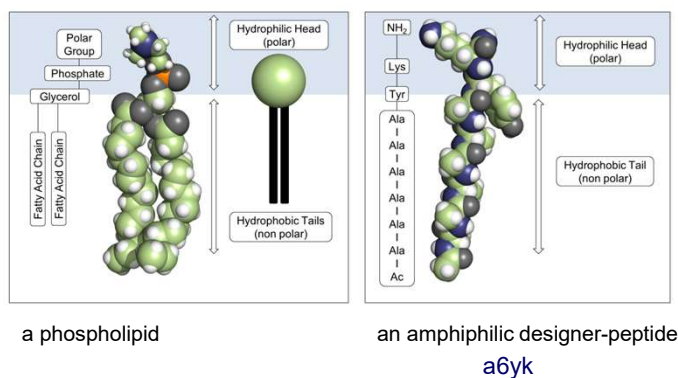
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE

Amphiphilic designer-peptides



68



Gazit, E. *Chem. Soc. Rev.* **2007**
Cherny, I.; et al., *Angew. Chem., Int. Ed.* **2008**

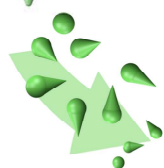
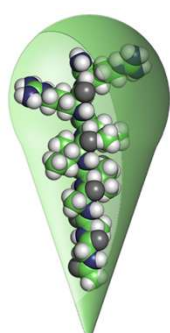
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

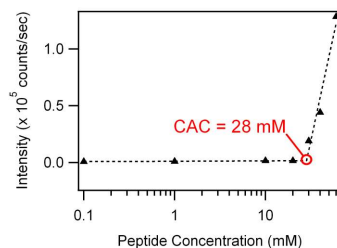
Anorganische
CHEMIE

Self-assembly

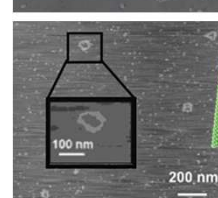
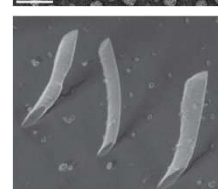
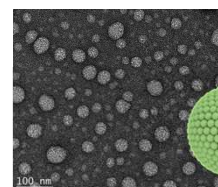
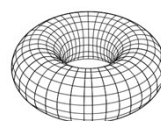
69



Spherical Micelles
Vesicles
Bilayers



Self-Assembly



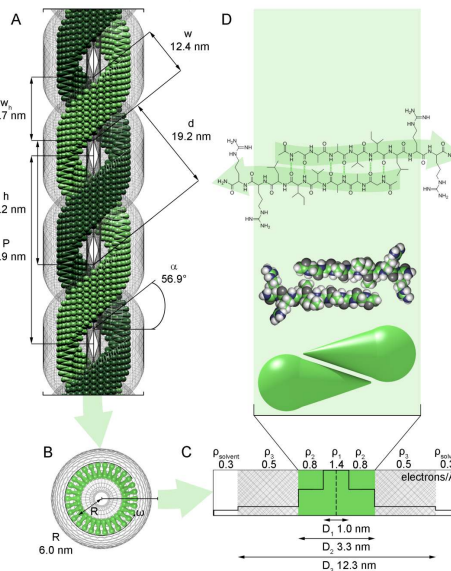
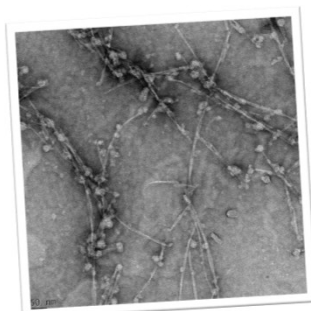
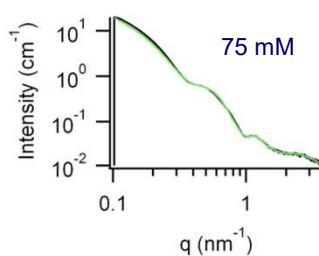
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE

It's a double helix!

70



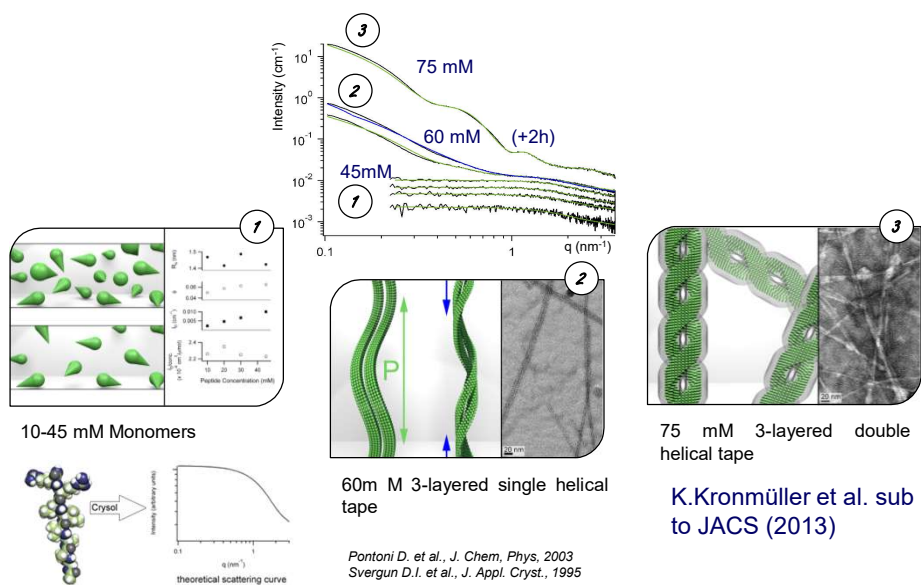
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE

The self-assembly process

71



SILS School 2026

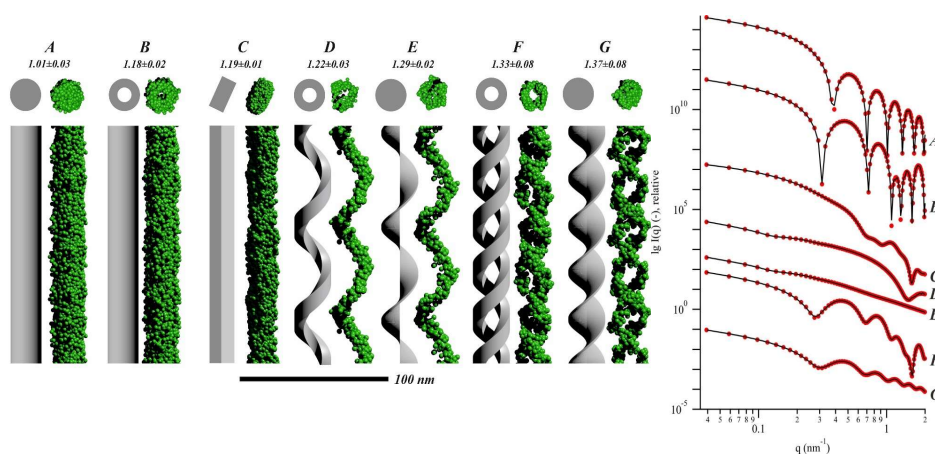
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

SAXS Software Development: SASHEL

72

Ab initio modelling of elongated structures (and globular structures)



M. Burian, H.A. IUCrJ (2018)

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

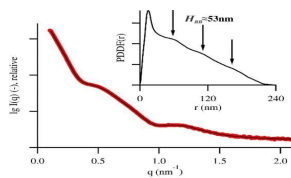
fAnorganische
CHEMIE

SAXS Software Development: SASHEL

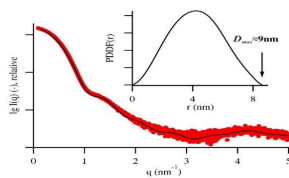
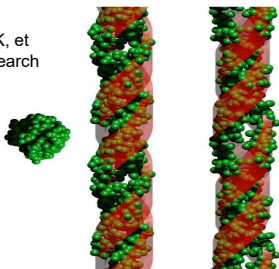


73

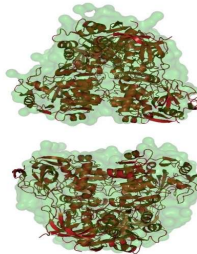
Ab initio modelling of elongated structures (and globular structures)



Kornmueller, K, et al. NanoResearch (2018)



Alcohol Dehydrogenase 1
Valentini E et al., Nucleic Acids Res. 43 (2015)



M. Burian, H.A. IUCrJ (2018)

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

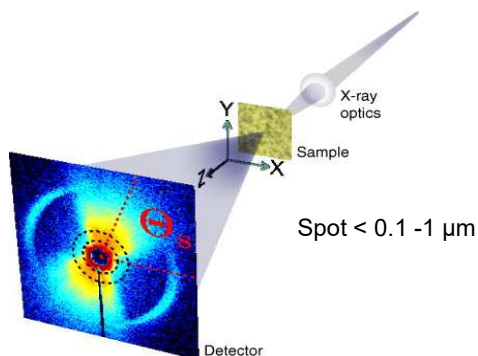
fAnorganische
CHEMIE



Scanning SAXS - Biomaterials

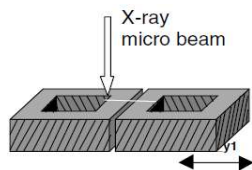


74



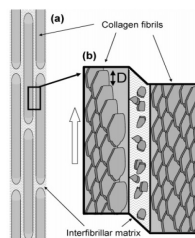
Pic. O.Bunk, et al. New J. Phys. 11 (2009) 123016

Silica-Sponges, Shells,
Tooth, Lobster, Worms,
Starch, Eyes.....,



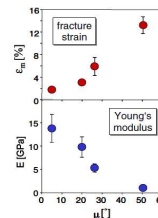
Bone

P.Fratzl



Wood

P.Fratzl



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



Scanning SAXS-Integral Parameters



75

Integrated Intensity

$$I = \int_{q \min}^{q \max} \int_{\chi_1}^{\chi_2} I(q, \chi) q^2 dq d\chi.$$

Porod Invariant

$$\begin{aligned} \tilde{I} &= \int I(\mathbf{q}) d^3q = \int_0^\infty q^2 dq \int_0^\pi \sin \psi d\psi \int_0^{2\pi} I(q, \psi, \chi) d\chi \\ &= 2\pi^2 \varphi_1 \varphi_2 (\Delta\rho)^2, \end{aligned}$$

T-Parameter

$$T = \frac{4}{\pi P} \int_0^\infty I(q) q^2 dq = 4 \frac{\varphi_1 \varphi_2}{\sigma} \quad \text{Porod (1951, 1952)}$$

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

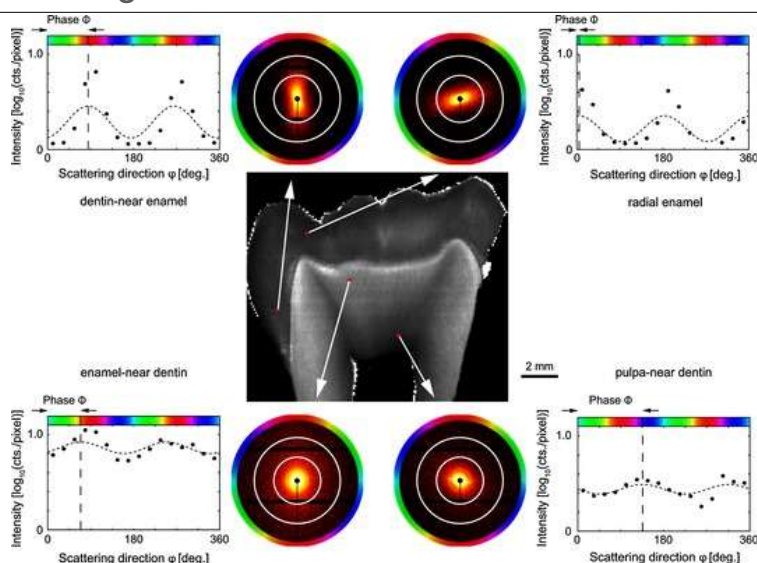
fAnorganische
CHEMIE



Scanning SAXS - Orientation



76



Geiser S. et al., Biointerphases
Journal for the Quantitative Biological Interface Data, 2012

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

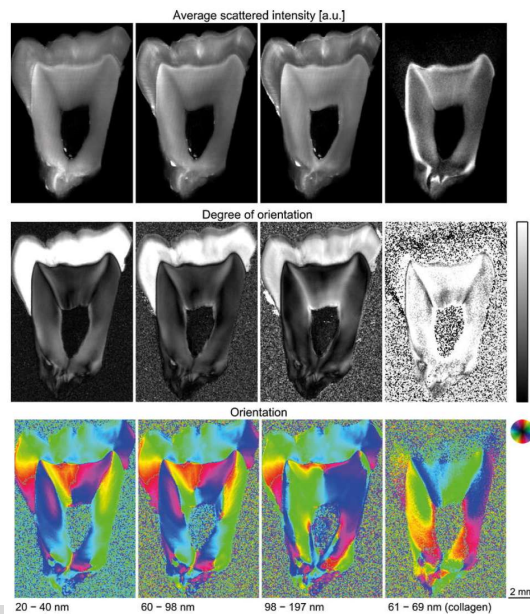
fAnorganische
CHEMIE



Scanning SAXS - Tooth



77



SILS School 2026

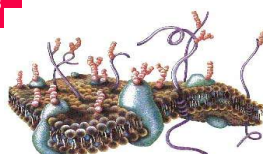
amenitsch@eletra.trieste.it

Anorganische CHEMIE

Liposomes and SAXS



78



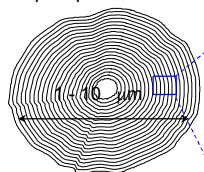
The boundaries of cells are formed by biological membranes, the barriers that define the inside and the outside of a cell.

Phospholipids are the major components of biological membranes that form the structural matrix into which proteins are imbedded.

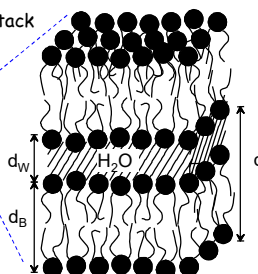


In aqueous solution:
self assembly into, e.g.,
unilamellar vesicles

Phospholipid Membrane Stack

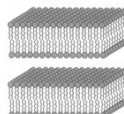


multilamellar vesicle:
LIPOSOME

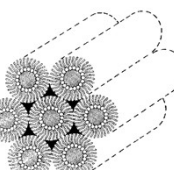


Lyotropic Phases

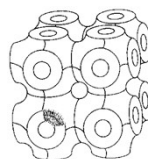
Bilayer



Micelle



Hexagonal Phase



Cubic Phase

SILS School 2026

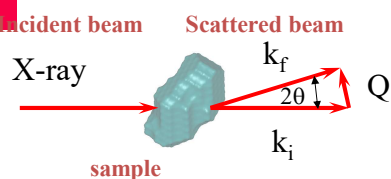
amenitsch@tugraz.at &
amenitsch@eletra.trieste.it

Anorganische CHEMIE

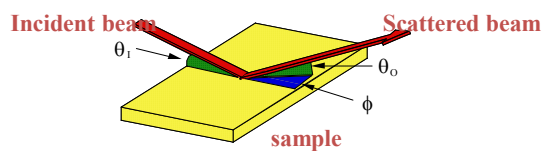
Small Angle Scattering - Surface Diffraction



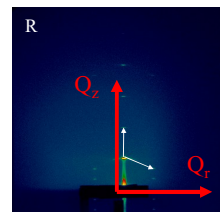
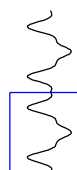
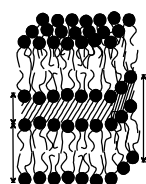
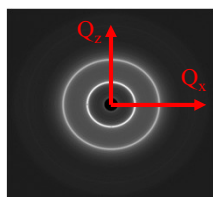
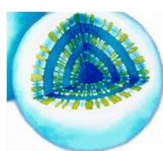
79



Small-Angle Scattering (Diffraction)



Grazing Incidence Small-Angle Scattering (GISAS) + Reflectometry



$$I(Q) = \left\langle \left| \int_V d^3r \cdot \rho(\vec{r}) \cdot \exp(-i \cdot \vec{Q} \cdot \vec{r}) \right|^2 \right\rangle$$

$$I(Q_z, Q_r) = \left\langle \left| \int_V d^3r \cdot \rho(\vec{r}) \cdot \exp(-i \cdot \vec{Q} \cdot \vec{r}) \right|^2 \right\rangle$$

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische CHEMIE

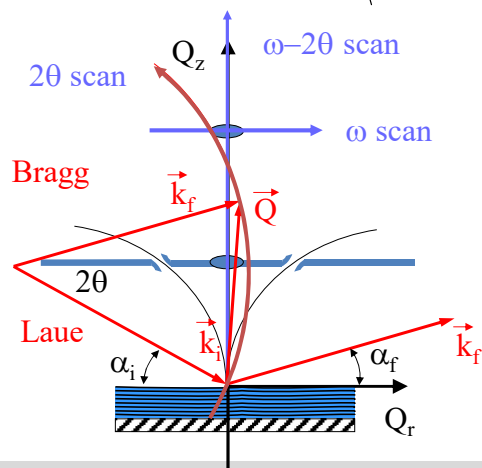
Distorted Wave Born Approximation



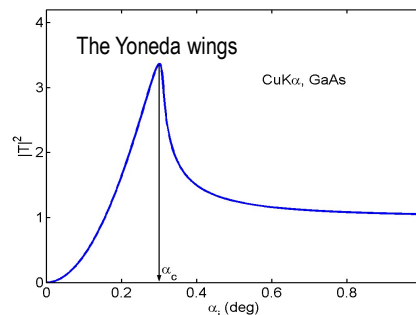
80

Vineyard (1982), Shinha et.al. (1988)

$$I(Q_z, Q_r) = |T_i(\alpha_i)|^2 \left\langle \left| \int_V d^3r \cdot \rho(\vec{r}) \cdot \exp(-i \cdot \vec{Q} \cdot \vec{r}) \right|^2 \right\rangle_r |T_f(\alpha_f)|^2$$



Refraction Effects



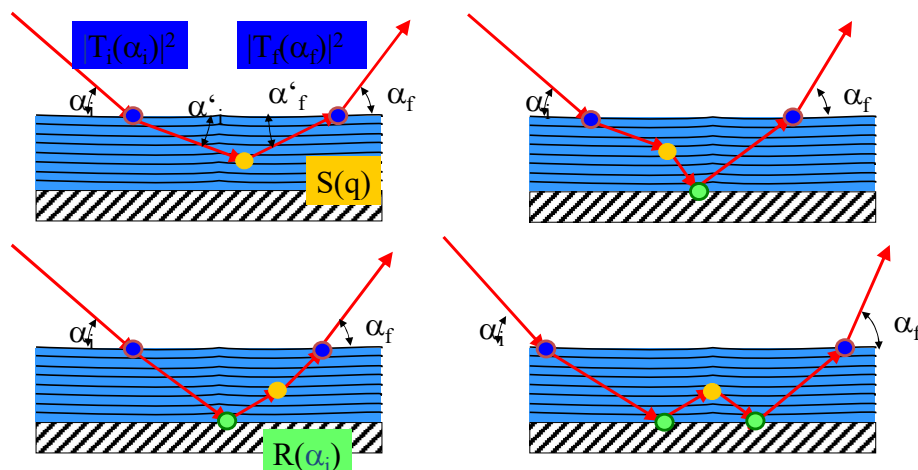
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische CHEMIE

„Higher Orders“ of DWBA

81



Lazzari R, ISGISAXS: program, J APPL CRYSTALLOGR 35: 406, (2002)

http://www.esrf.fr/computing/scientific/joint_projects/IsGISAXS/igisaxs.htm

M.P.Tate et al., J.Phys.Chem, 2006

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Distorted Wave Born Approximation

82

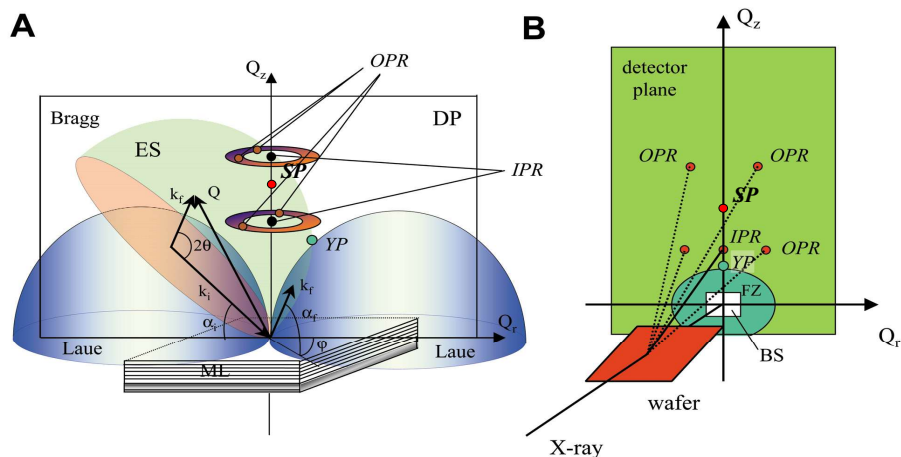
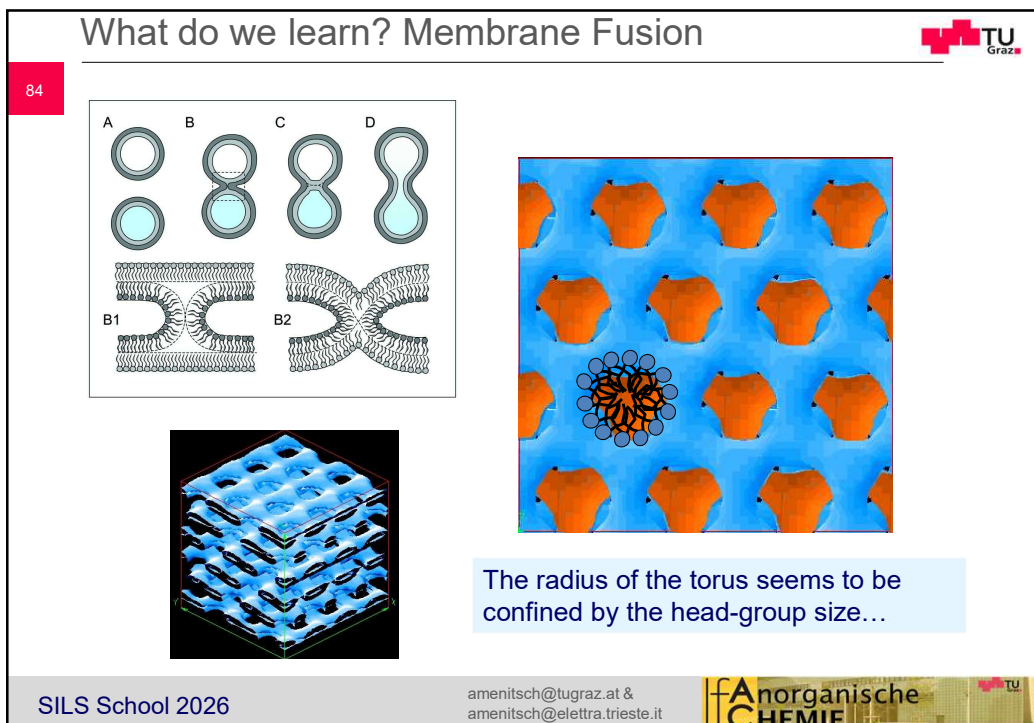
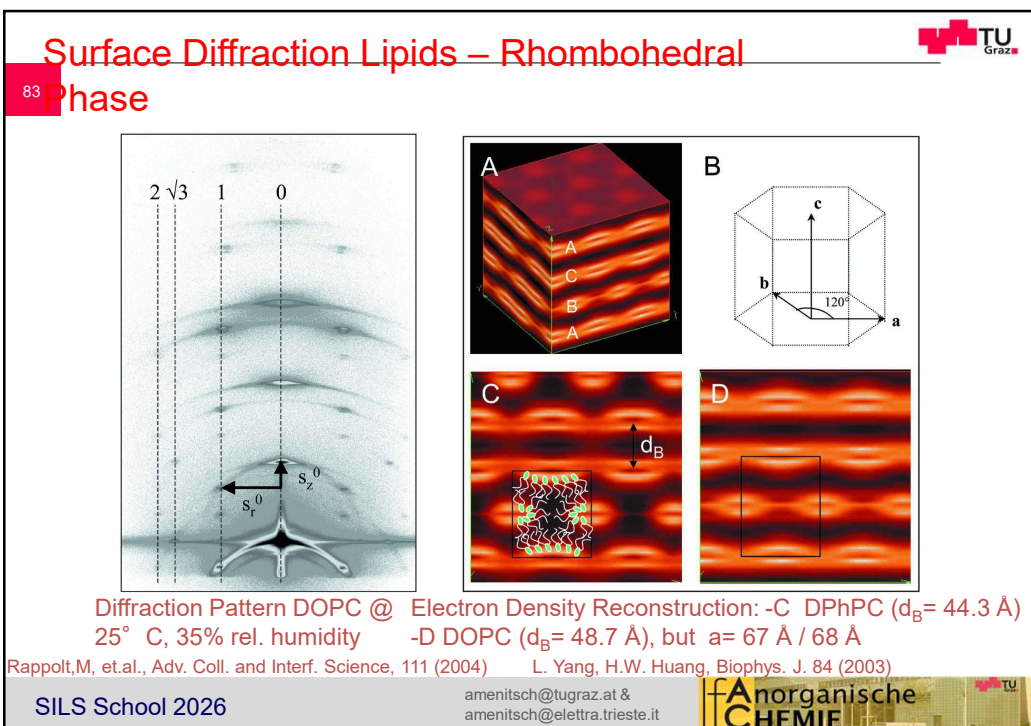


Fig. (A) the scattering geometry in reciprocal space. (B) Scattering geometry in real space. The abbreviations are: (ES) Ewald sphere, (DP) diffraction plane, (OPR) out-of plane reflections, (IPR) in-plane reflections, (ML) multi-layer, (FZ) forbidden zone, (BS) beam stop.

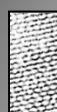
SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE



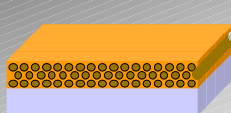
Sol-gel chemistry
+
surfactant mesophase
↓
Self-assembly
Mesostructured hybrids
↓
Treatment
Mesoporous materials with organised porosity



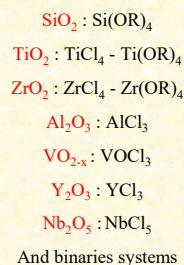
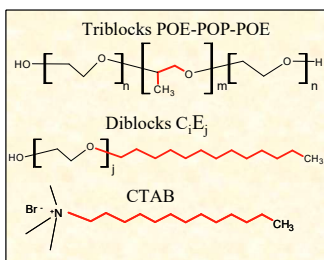
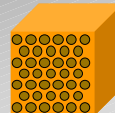
Particles made by aerosols



Films and fibres made by liquid deposition



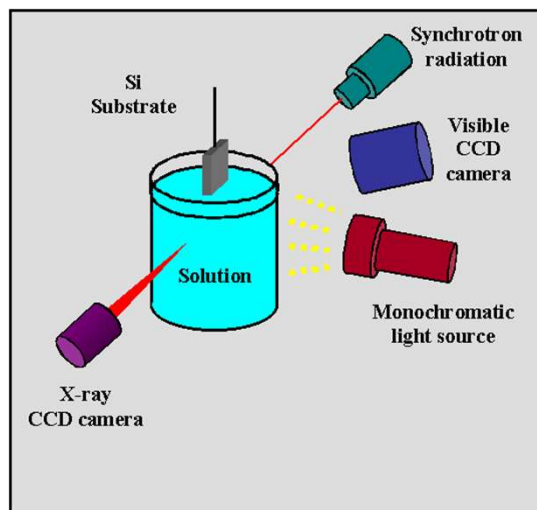
Monoliths made controlled evaporation



amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

f **A**norganische
CHEMIE

Film mesostructure



Film thickness profile

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Surface diffraction: Formation of aligned mesoporous thin films



87

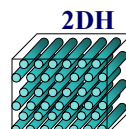
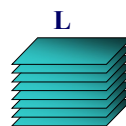
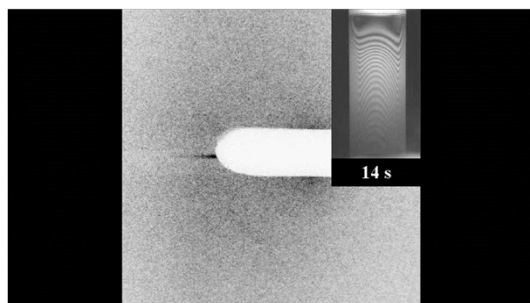
CTAB / Si = 0,18

H₂O / Si = 5

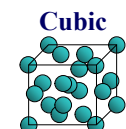
HCl / Si = 0.15

Ageing time

Relative Humidity



P6m



Pm3n

Im3m

Grosso D, et.al., CHEMISTRY OF MATERIALS 14, 931,(2002)

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE



The Modulable Steady State



88

E. Cagnol et al., J. Mater. Chem., 2002

1 Quantity of surfactant

FIXED

2 Quantity of Inorganic Precursor

Evaporation of EtOH
Preventing condensation
Locking the mesostructure
Induced by self-assembly
(time dependent
induced by self-assembly)

Process: Dip-Coating
"The Evaporation induced self assembly"

3 Quantity of H₂O

Depends the relative humidity with the dip-coater

Initial solution

Surfactant + H₂O + EtOH + HCl + Inorg. Precursor

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE



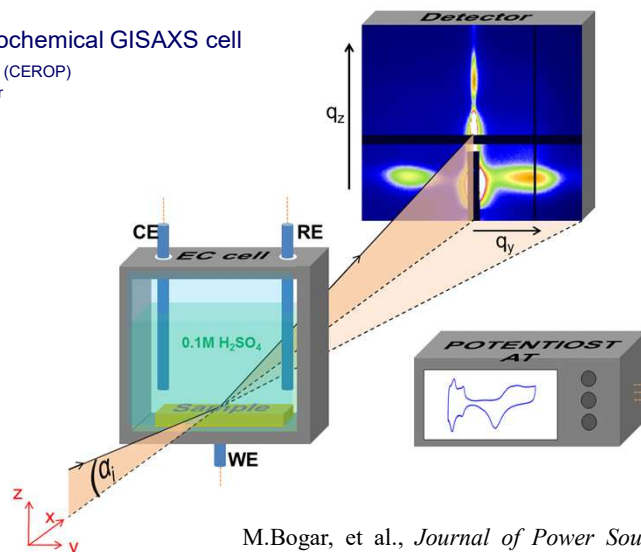
Electrochemistry - GISAXS



89

-Electrochemical GISAXS cell

M.Bogar (CEROP)
P.Wieser



M.Bogar, et al., *Journal of Power Sources*
(2020) 477, 229030.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

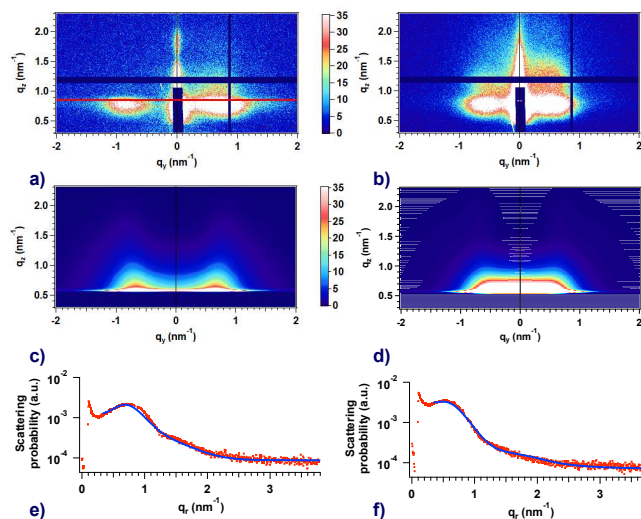
fAnorganische
CHEMIE



GISAXS: Pt/Ni nanocatalyst fuel cell



90



LAYER GEOMETRY:
sandwiched islands

FORM FACTOR:
random spheroid,
H/D constant

SIZE DISTRIBUTION:
Log Norm

STRUCTURE FACTOR:
Perkus-Yevick

FORM FACTOR:
D: 4.3 nm
FWHM: 3.7 nm
H/D: 5

STRUCTURE FACTOR:
A/D: 2.95
eta: 0.127

FITGISAXS - D. Babonneau, J.Appl.Cryst, (2010)

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

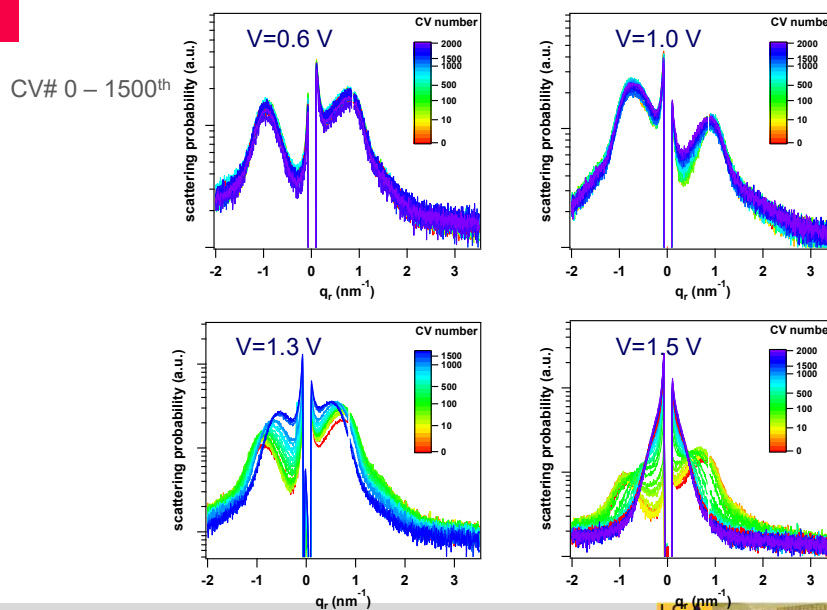
fAnorganische
CHEMIE



GISAXS: Pt/Ni nanocatalyst fuel cell



91



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

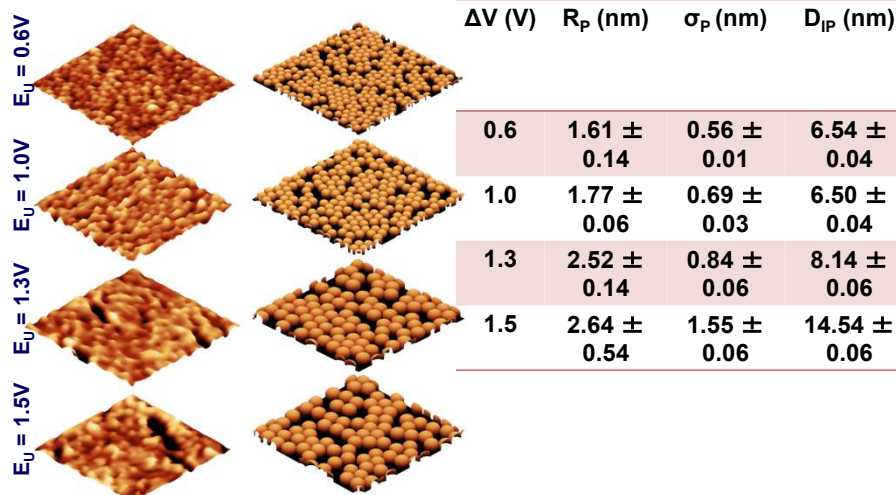
Anorganische
CHEMIE



Sketch of the Model - GISAXS: Pt/Ni nanocatalyst



92



I. Khalakhan, et al., *ACS Applied Materials and Interfaces* (2020) 12, 17602.

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE



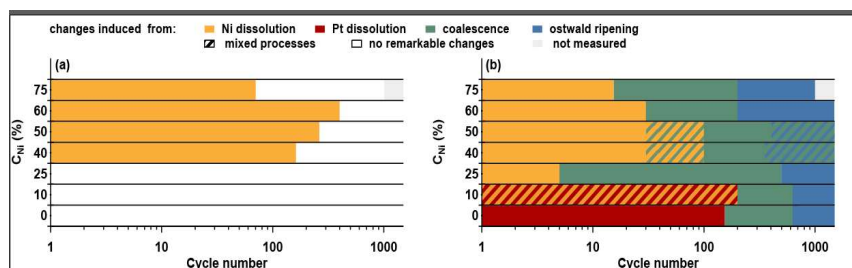
Pt_xNi_{1-x} Dependence - GISAXS: Pt/Ni nanocatalyst



93

1.0 V_{RHE}

1.3 V_{RHE}



Ni/Pt dissolution

Coalescence

Ostwald ripening

Initial state

M.Bogar et al.
ACS Catalysis (2021)

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

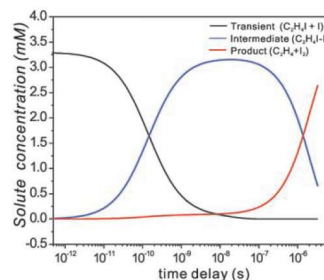
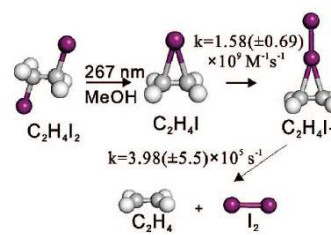
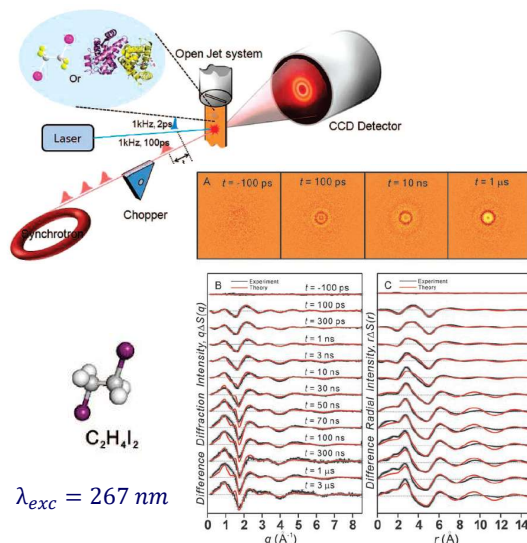
Anorganische
CHEMIE

Pump Probe: Transient solution scattering



94

Taken from: H.Ihee, et al. Science **309**, 1233 (2005).



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

Anorganische
CHEMIE

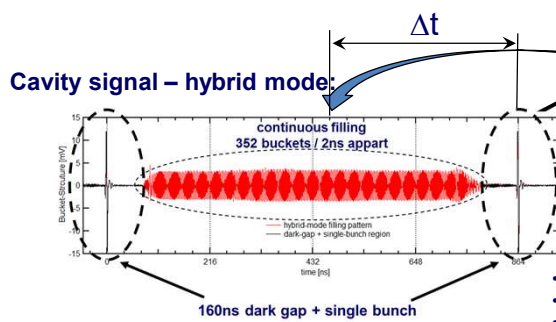
Pump Probe: Implementation



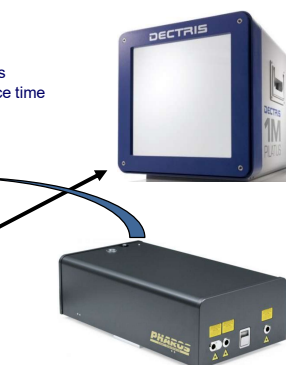
95

Elettra storage ring specifications

- 80 ps x-ray pulses
 - 500 MHz cavity
 - 432 bucket slots
- one pulse every 2ns
→ 864ns circumference time



(End September 2018)



Pharos 20W Nd YAG: Laser

- Pulse width < 230 fs
- Wavelength Harmonics of 1030nm
- Chose-able repetition rate up to 600 kHz
- 100μJ pulses (@1030nm)
- Time-jitter < 5ps



SILS School 2026

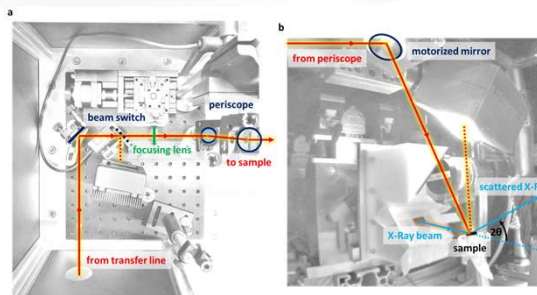
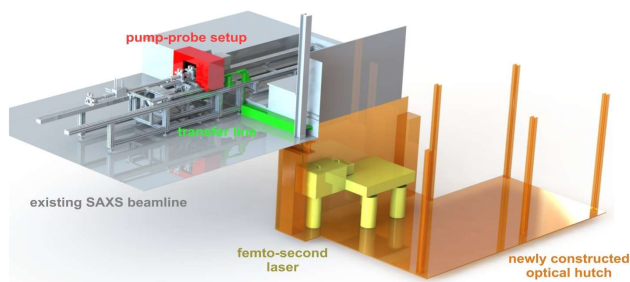
amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Pump Probe



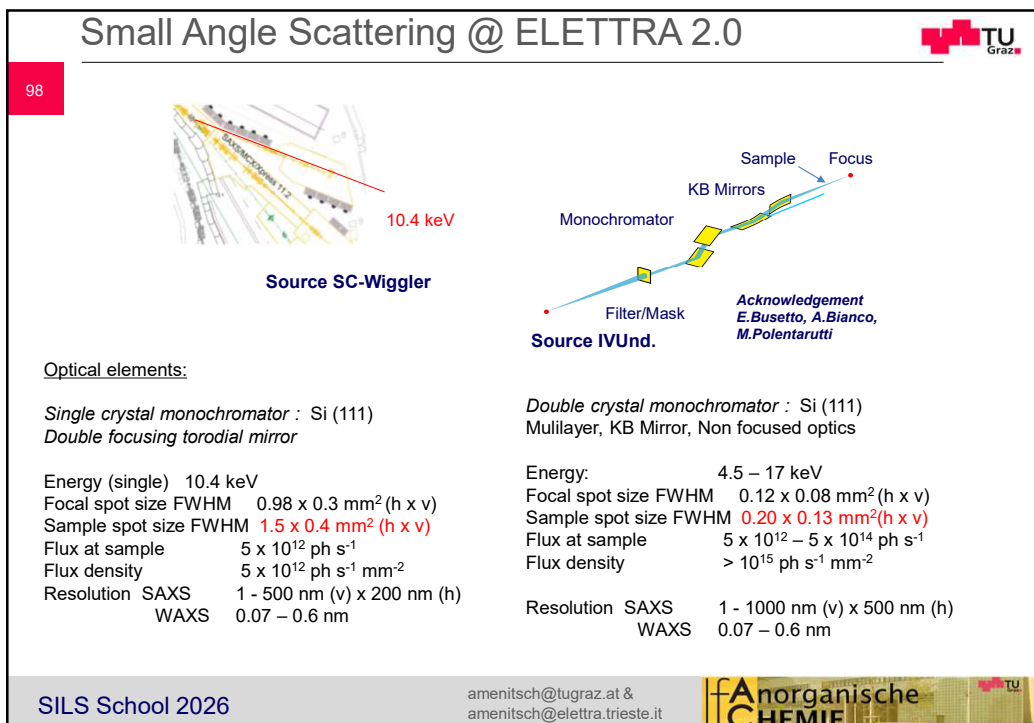
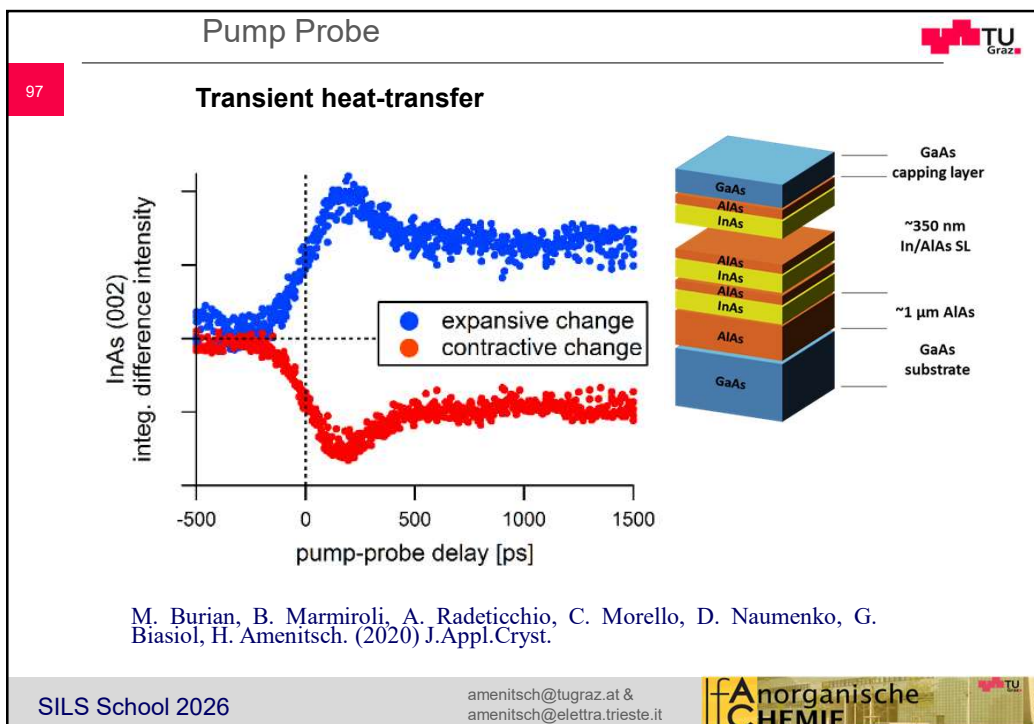
96



SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

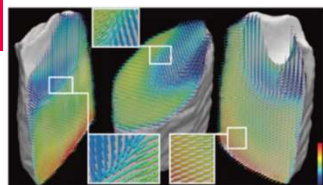
fAnorganische
CHEMIE



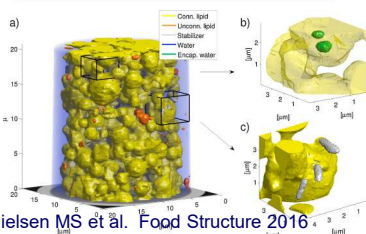
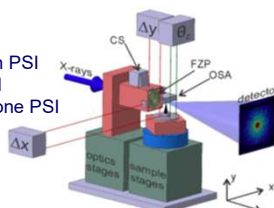
Current Science Development – ELETTRA 2.0



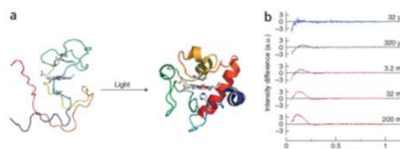
99



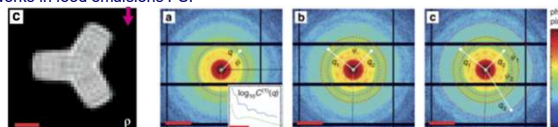
Schaff et al. Nature 2015
3D SAXS tomography tooth PSI
Liebi et al. Nature 2015 PSI
3D SAXS tomography of bone PSI



Nielsen MS et al. Food Structure 2016
Pythagoric X-ray computed tomography of extended colloidal networks in food emulsions PSI



Cammerata M. et al. Nature 2008
Pump probe WAXS Cyt-c. ESR



Pedriani et al. Nature com. 2013
2D cross correlation PSI

0.16 1/nm

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE

Conclusion



100

PART I:

- Introduction to the Theory ("Graz School")
- From Experiments to Real Space
- Bio-SAXS ("Hamburg School")

PART II:

- Examples:
 - Chemistry
 - Hierarchical Materials
- Grating Incidence SAXS ("no school")
 - Biomembranes
 - In situ Chemistry
 - In operando Electrochemistry
 - Pump-Probe



www.elettra.eu

YouTube SAXS & CERIC-ERIC

SILS School 2026

amenitsch@tugraz.at &
amenitsch@elettra.trieste.it

fAnorganische
CHEMIE