

Photon Density Wave Spectroscopy

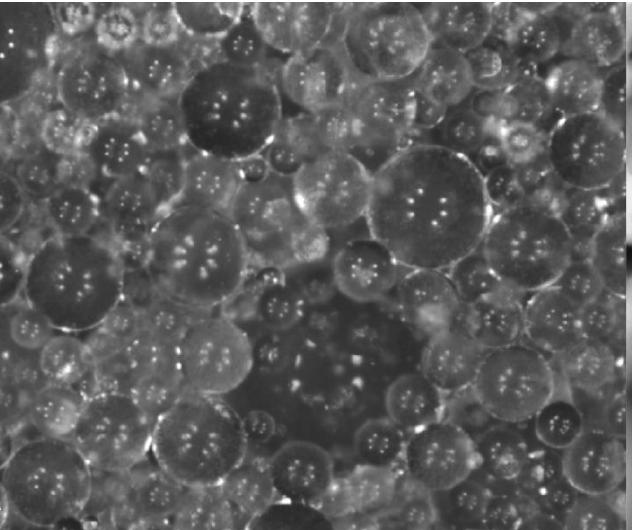
Potsdam, 15.11.2021

Dr. Marvin Münzberg

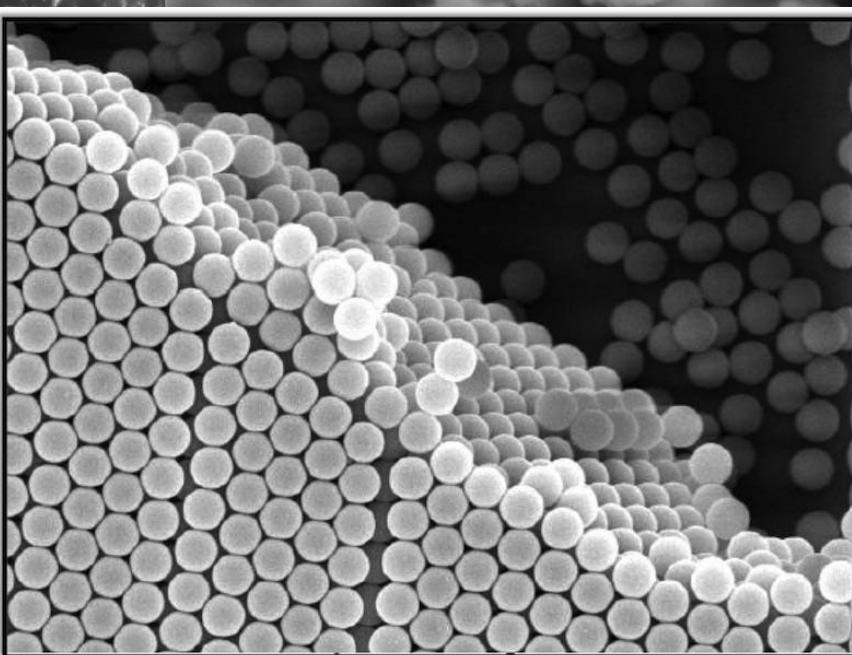
University of Potsdam, Physical Chemistry – innoFSPEC Potsdam, Applied
Analytical Photonics

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Bildquellen: guardianlv.com, alleideen.com, desy.de

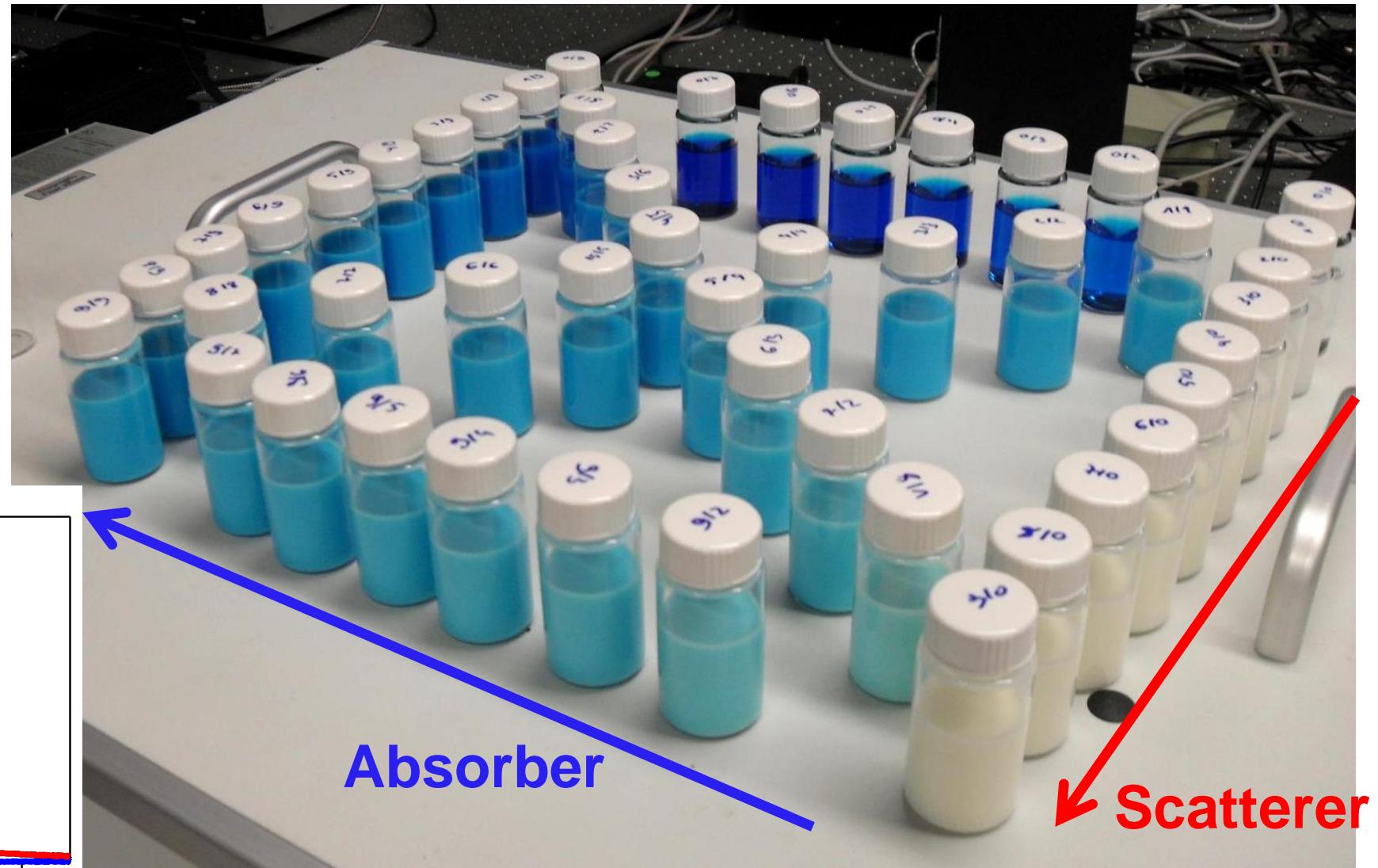
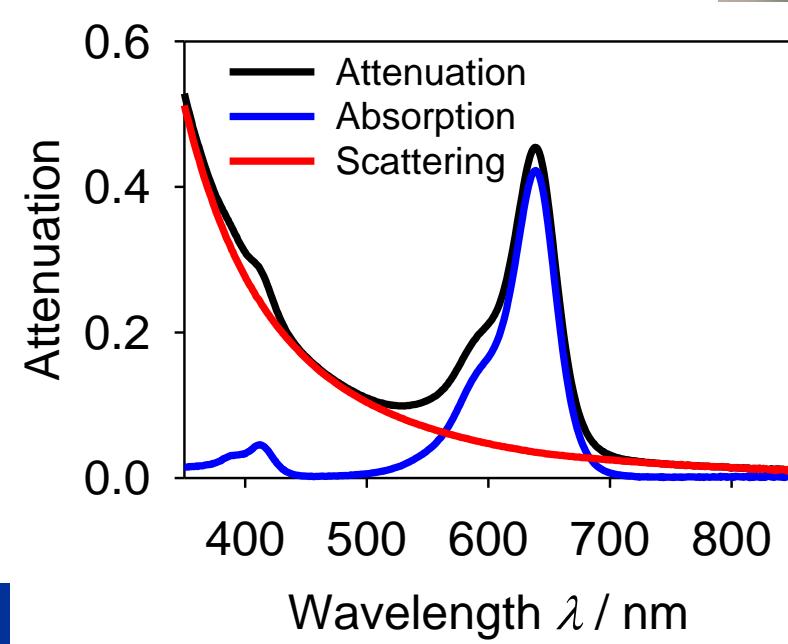
P. Werner, **M. Münzberg**, R. Hass, O. Reich, Analytical and Bioanalytical Chemistry, 09, S. 807-19, 2017



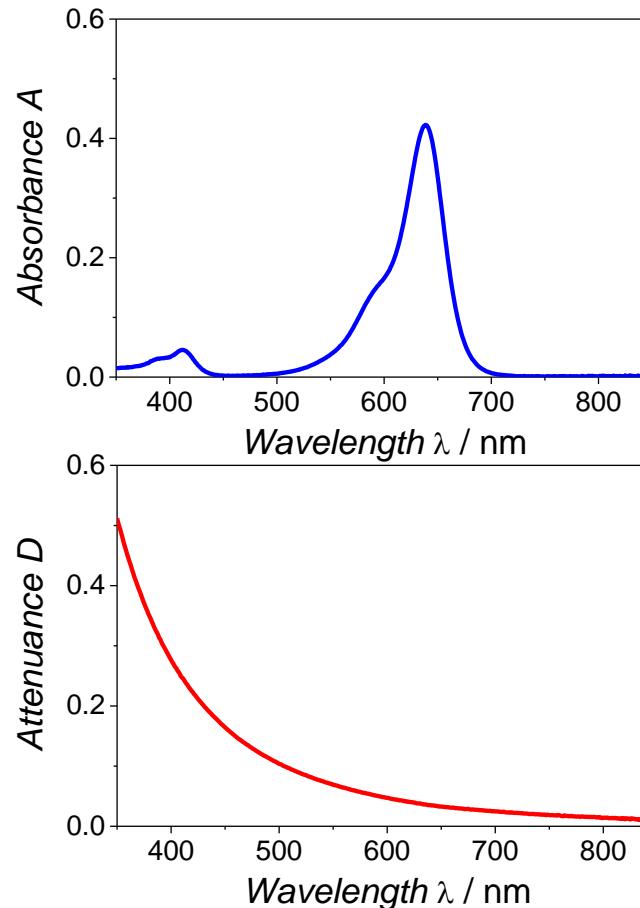
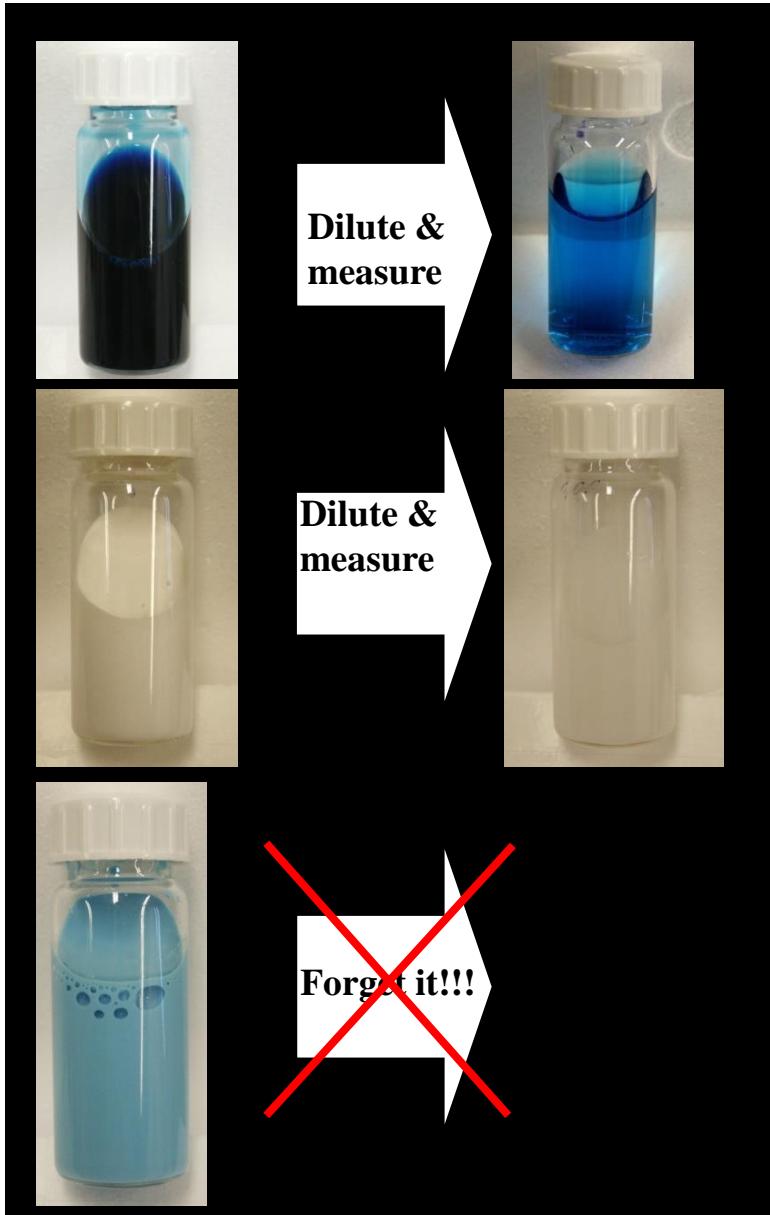
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Light absorption and scattering



Absorption & single scattering



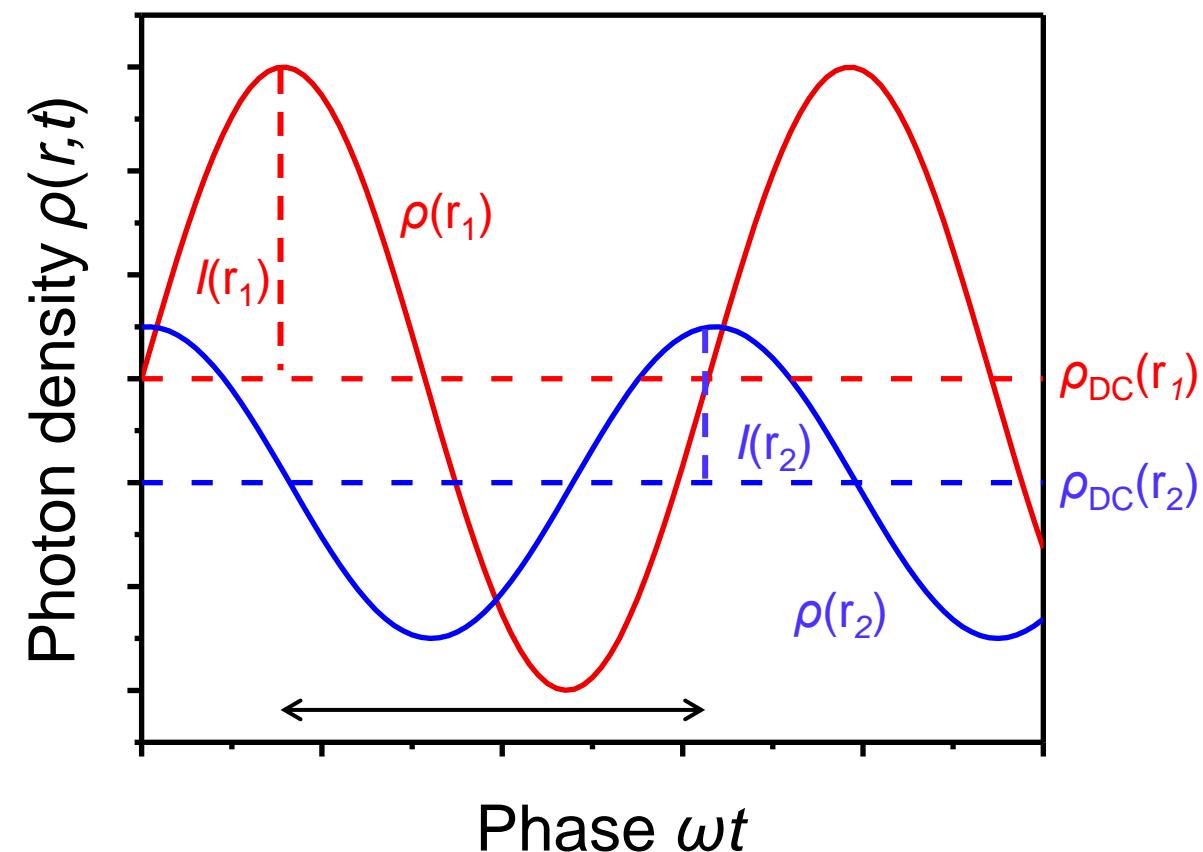
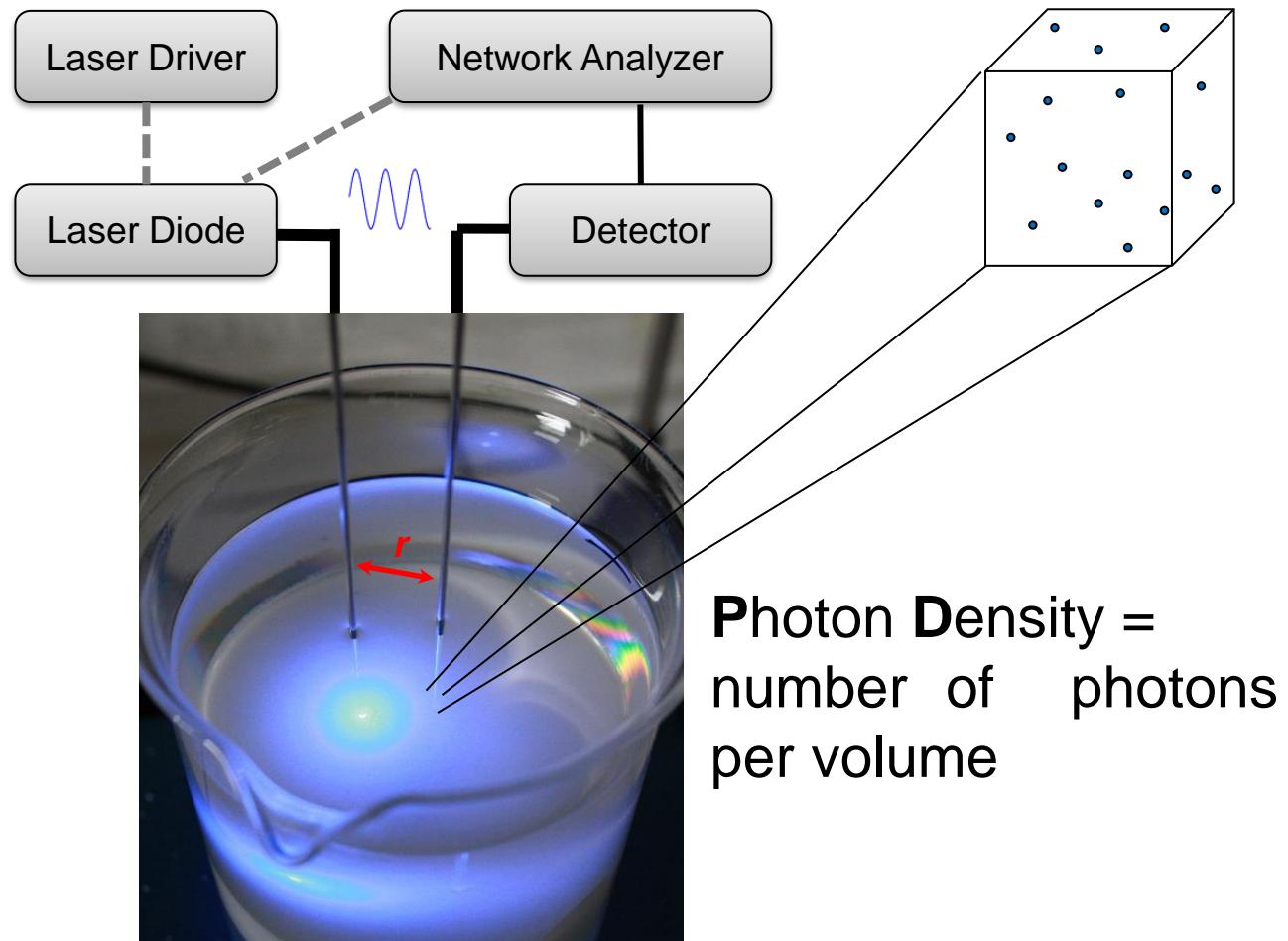
$$A = \mu_a l$$
$$= \epsilon_a c l$$

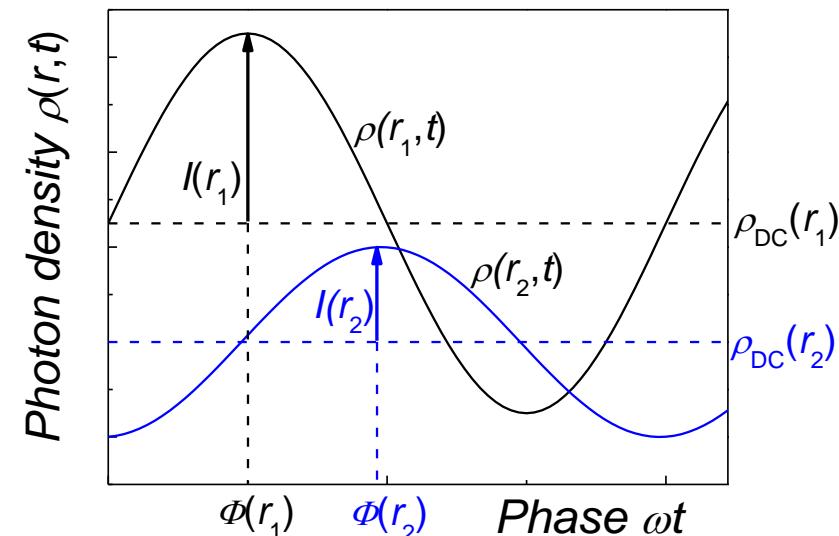
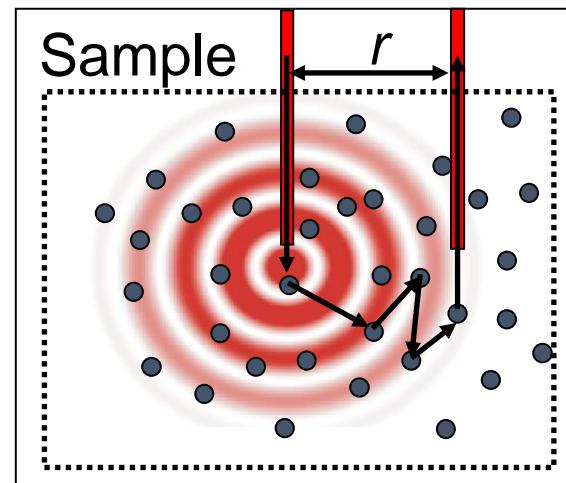
$$D = \mu_s l$$
$$= \epsilon_s c l$$

~~$$D = \ln \frac{I_0}{I} = [\mu_a + \mu_s]z$$~~

No linear correlation

Photon Density Wave(PDW)-Spectroscopy





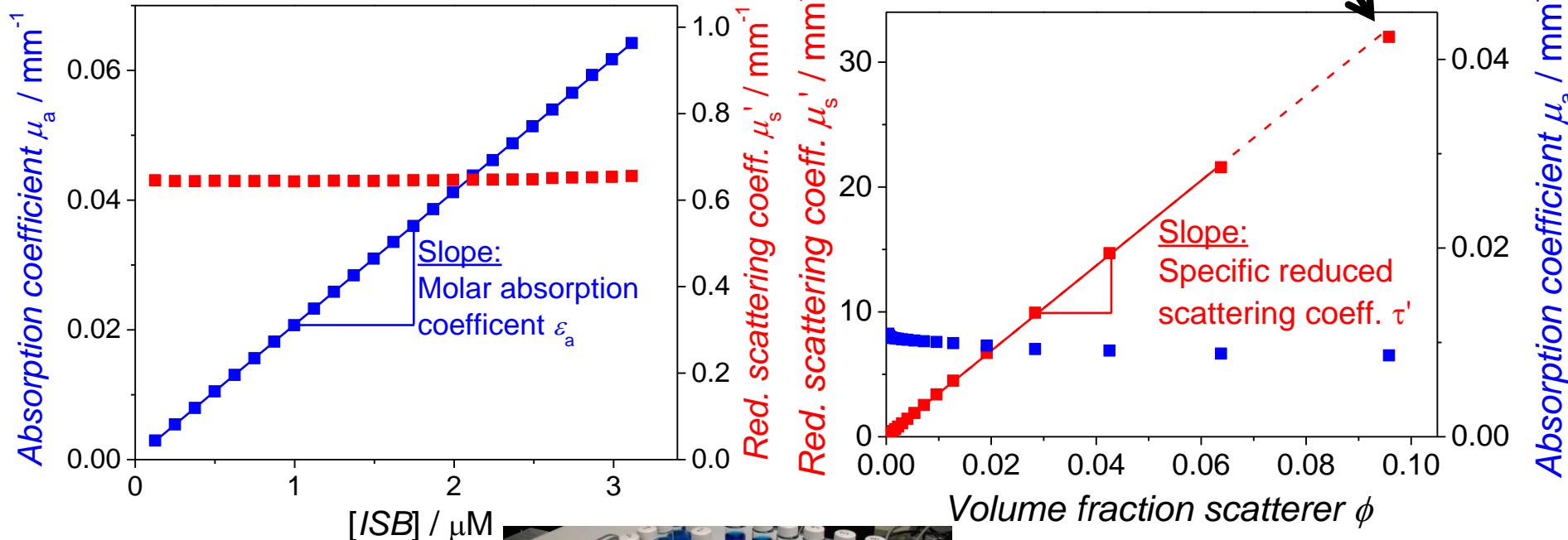
$$\text{Photon density: } \rho(r,t) = \underbrace{\frac{\rho_{DC}^0}{r} \exp[-k_{DC}r]}_{\text{const. in time}} + \underbrace{\frac{\rho_{AC}^0}{r} \exp[-k_I r] \cos[\omega t - k_\phi r]}_{\text{Intensity } I(r,\omega) \text{ Phase } \Phi(r,\omega)}$$

$$\text{Int.-/Phase coeff.: } k_{I/\Phi} = \sqrt{\frac{3}{2} \left\{ \sqrt{\left[\left[\frac{\mu_a}{3} + \mu_s' \right]^2 + \frac{\omega^2}{c^2} \right] \left[\mu_a^2 + \frac{\omega^2}{c^2} \right]} \pm \mu_a \left[\frac{\mu_a}{3} + \mu_s' \right] \mp \frac{\omega^2}{c^2} \right\}}$$

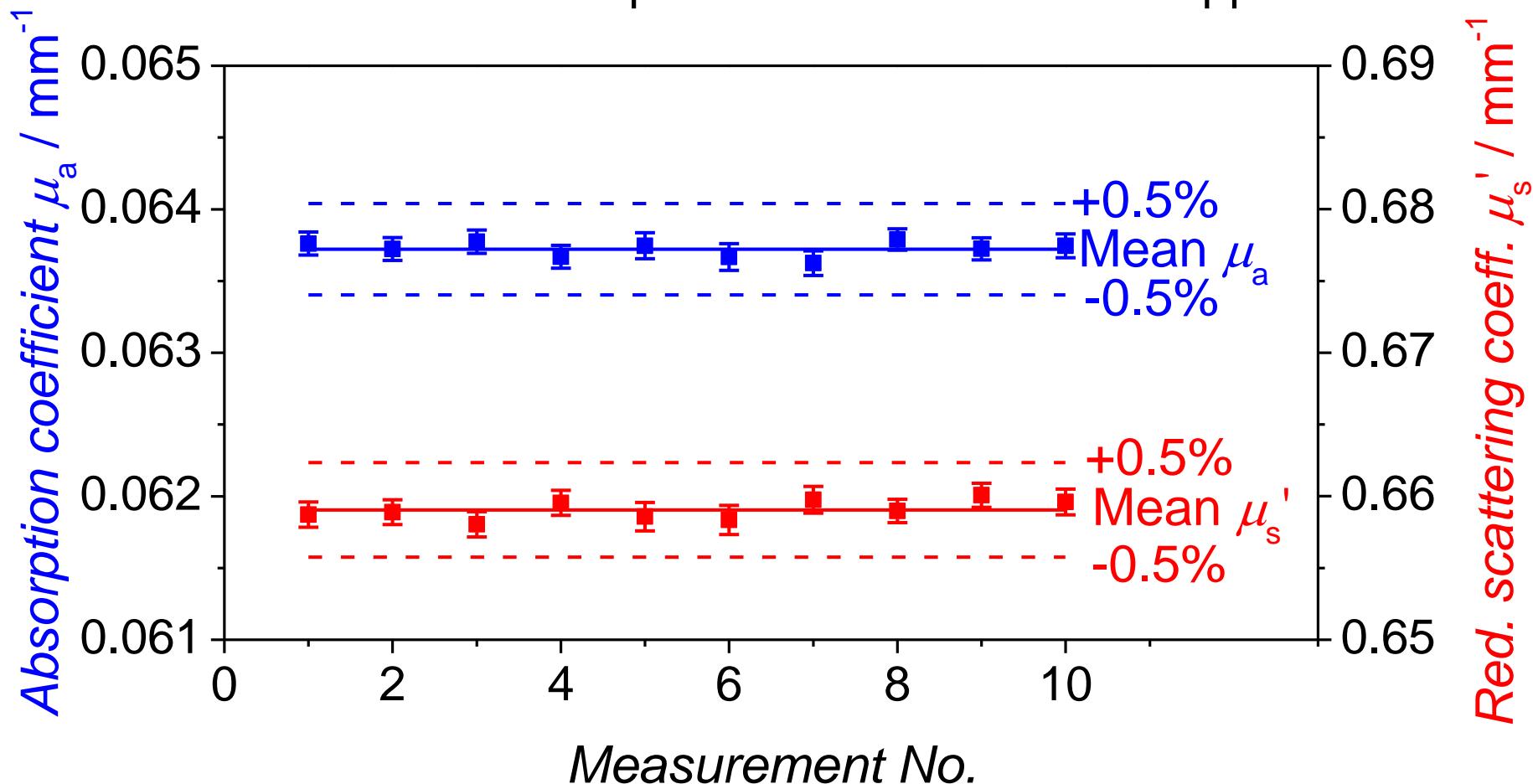
Absorption & scattering properties independently accessible!

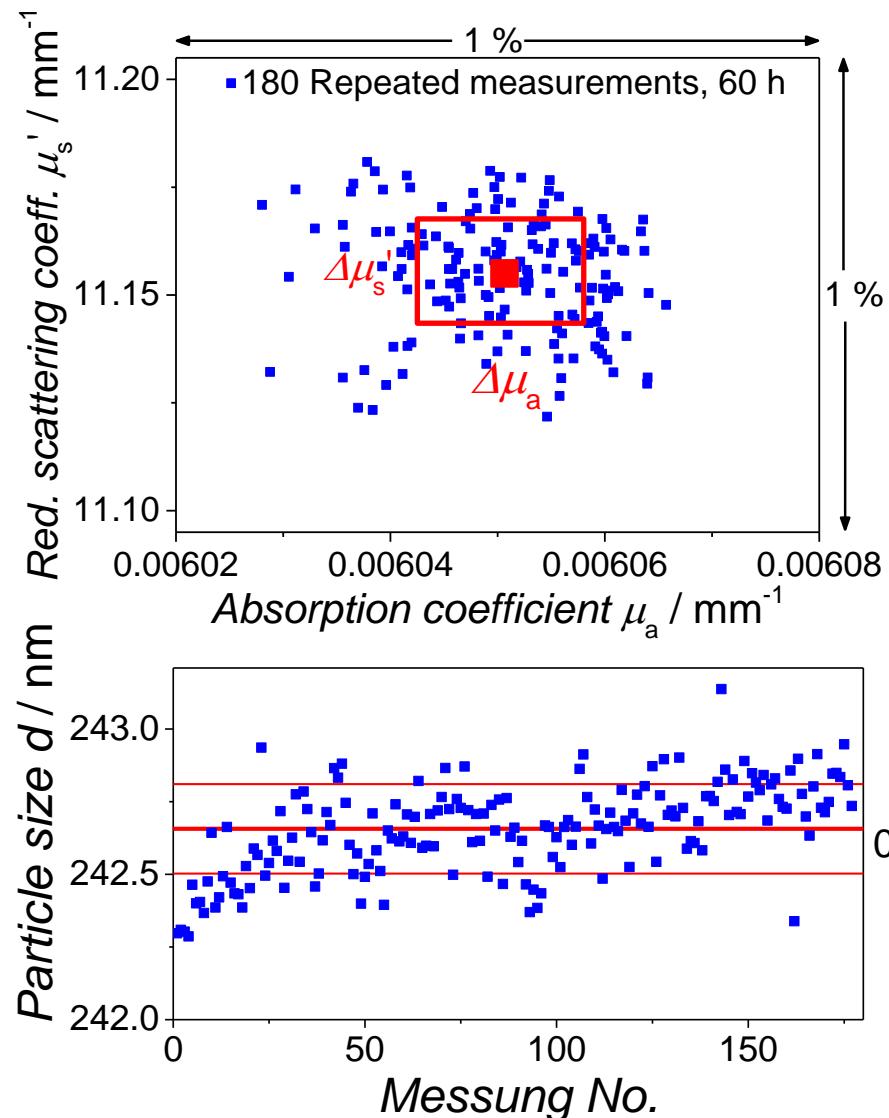
- Determination of concentration (via absorption)
- Determination of particle size (via scattering)

1 cm-cuvette:
 $D = 3000!!!$
 $D_{\max}(\text{Turbidim.}) = 3$



- „Precision“ often far better than 1 %, good error estimates
- Translates to precision of:
 - particle size = sub nm
 - abs. concentration = sub nM
 - particle vol. fraction = sub ppm





Precision of optical coefficients:

$\Delta\mu_s' : 1.4 \times 10^{-2} \text{ mm}^{-1}$ (0.12%)

$\Delta\mu_a : 8.4 \times 10^{-6} \text{ mm}^{-1}$ (0.14%)

equals [Abs] of 400 pM or

equals absorption length of 120 m!

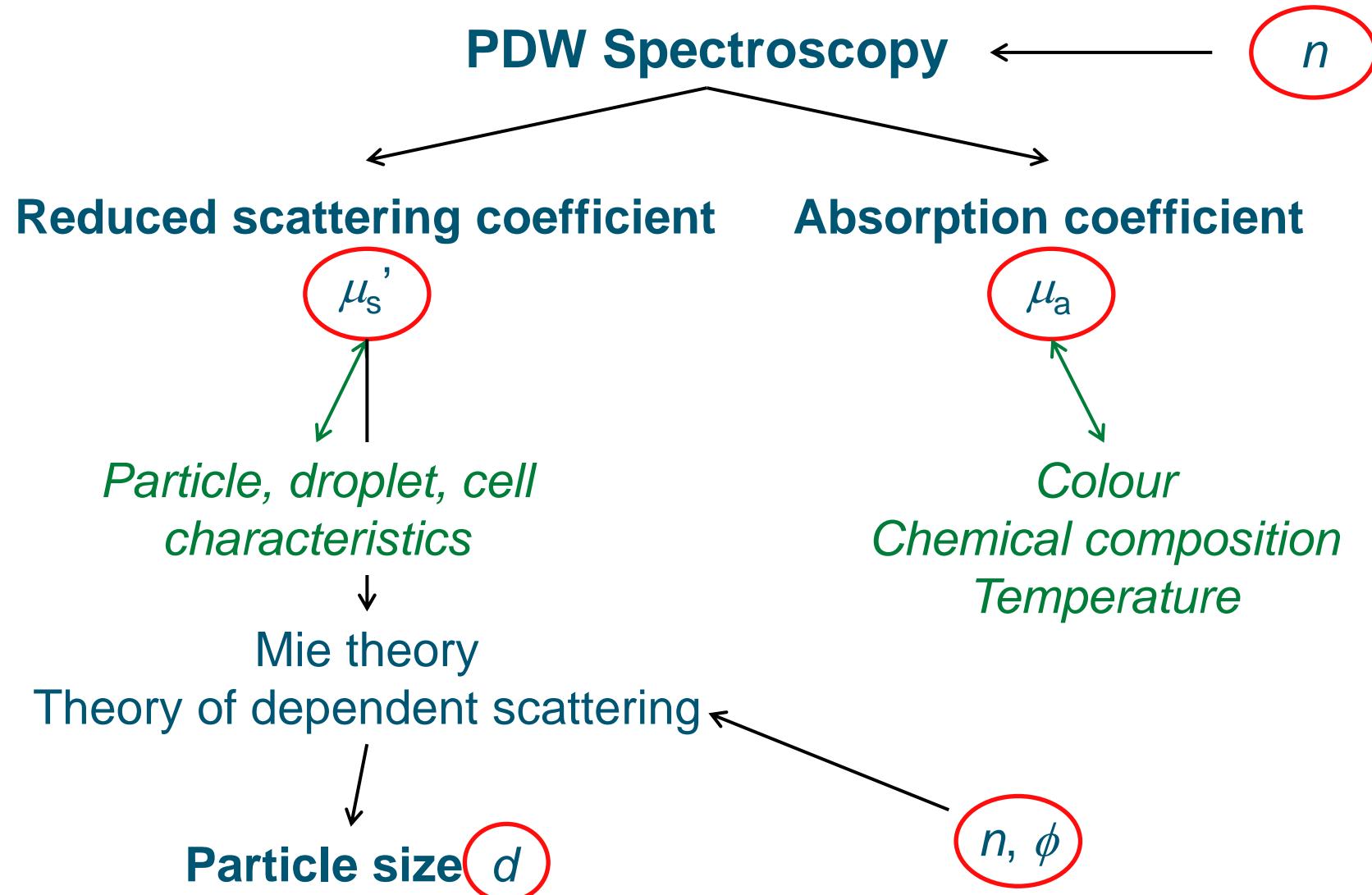
Precision particle size:

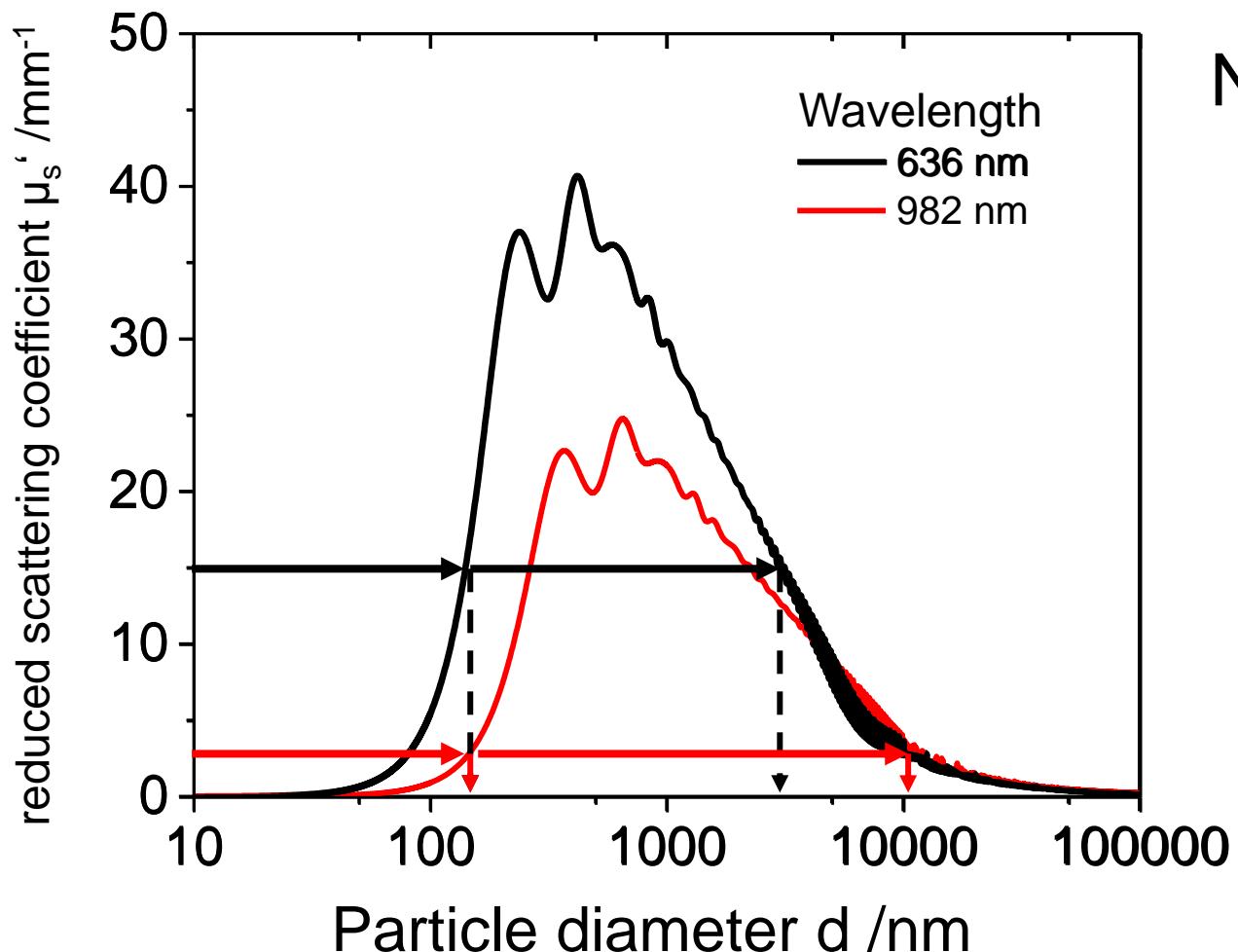
$\Delta d : 0.15 \text{ nm}$ (0.06 %)

equals a single C-C-bond length!

Important:

Absorption and reduced scattering coefficients not correlated!

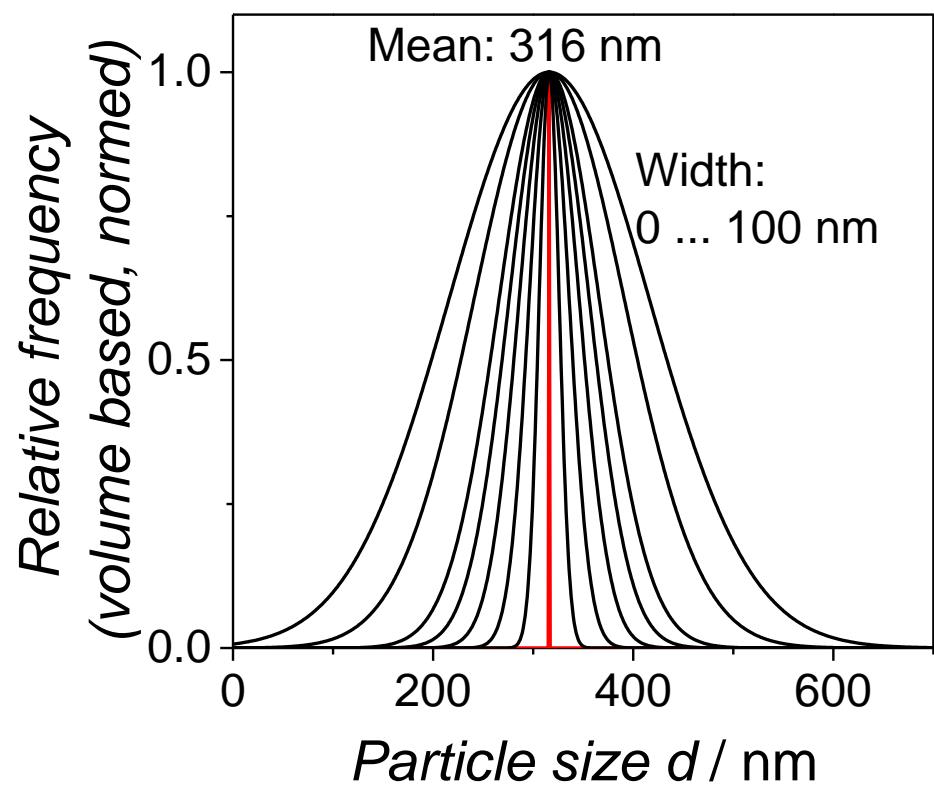




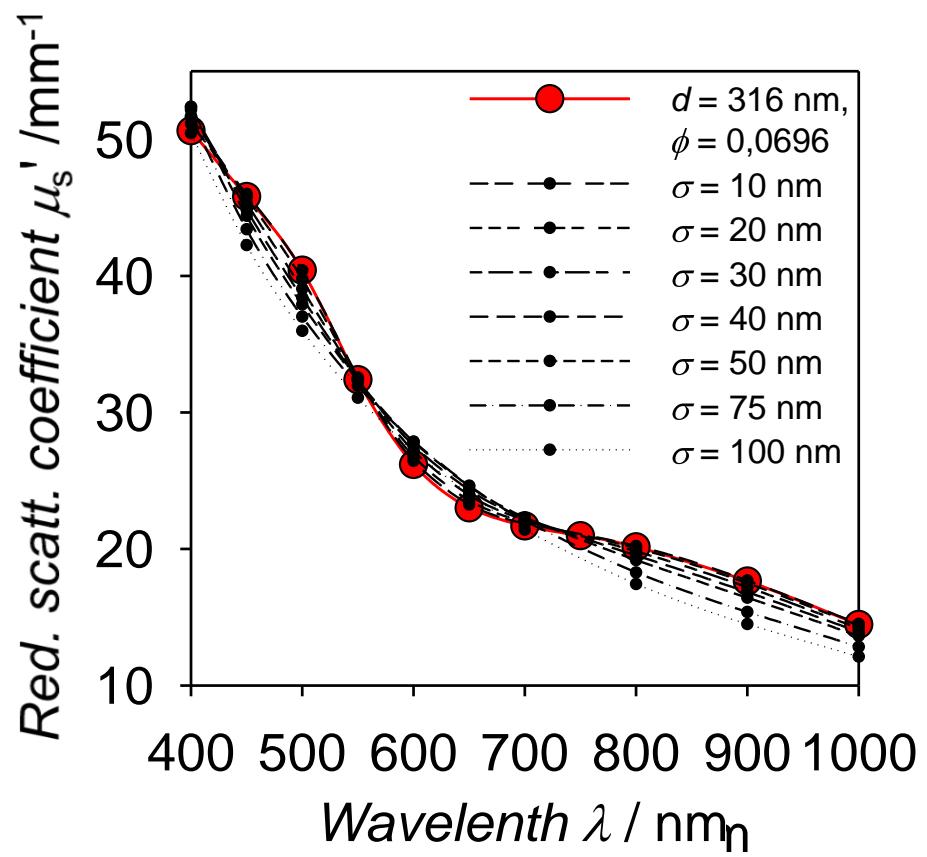
Number of Wavelength λ

1	no choice
2	average size
many (500-1000 nm)	distribution

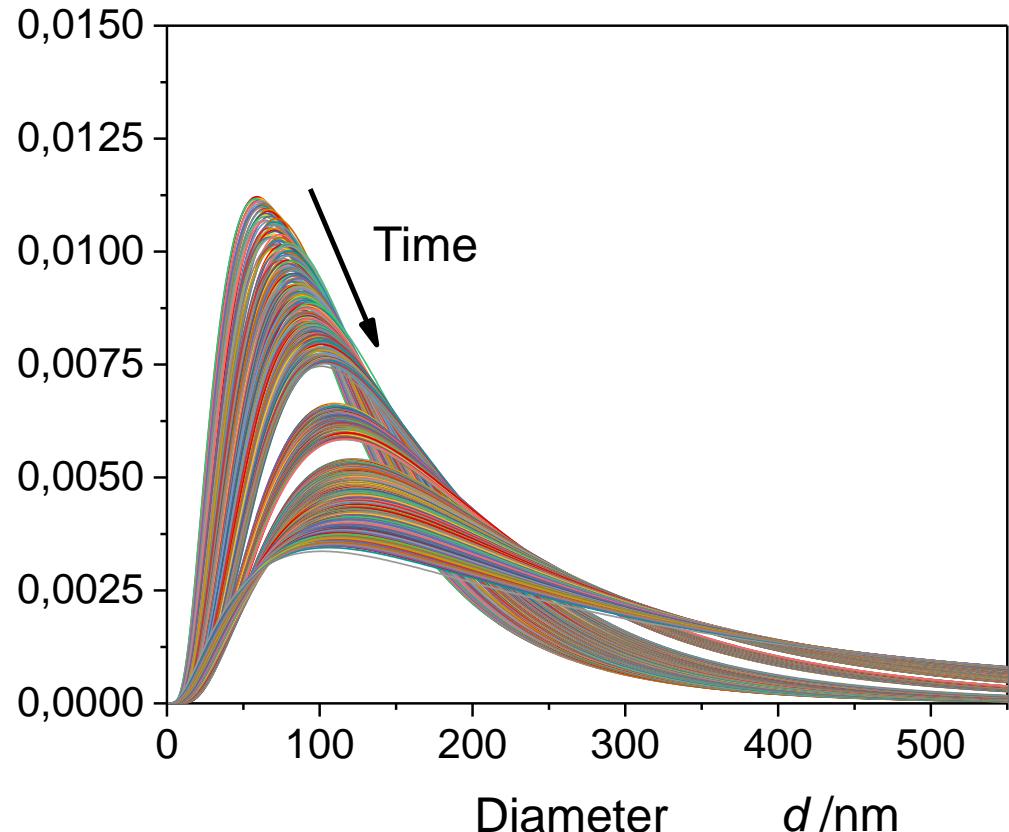
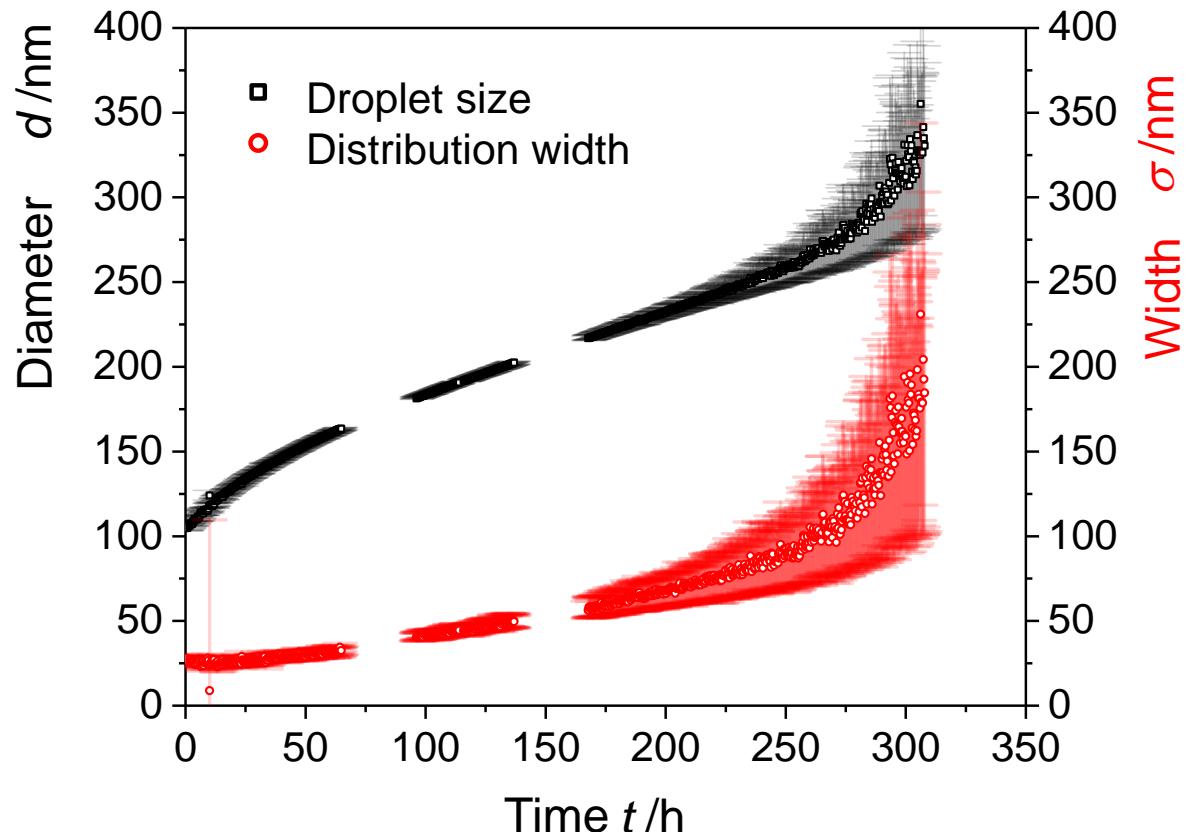
Parameterized PSDs
(here: volume based
Gaussian distribution)

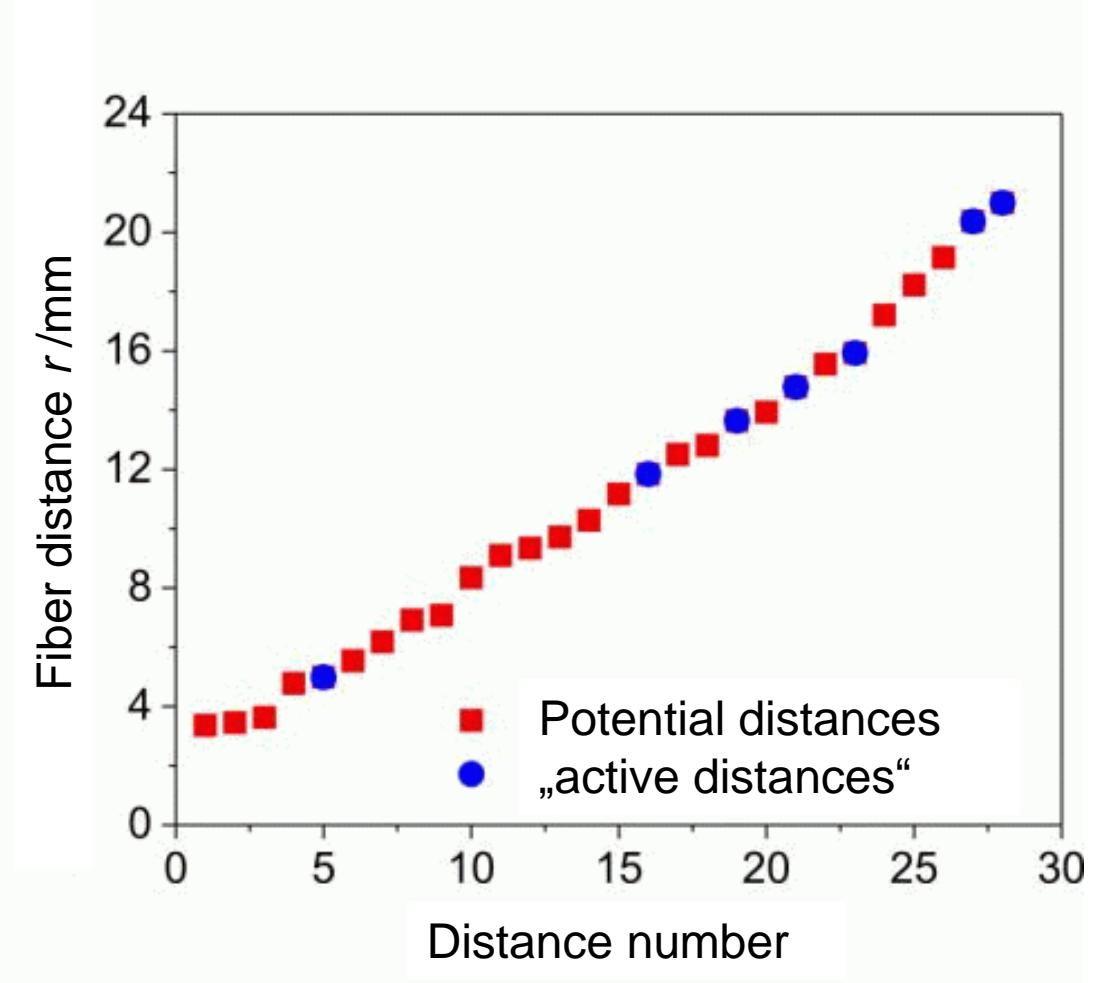
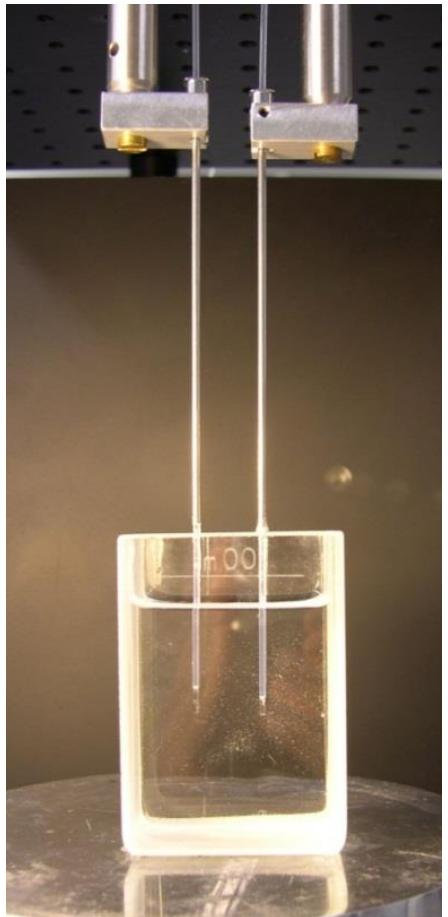


Calculation of spectral dependency of μ_s'



Particle / Droplet sizing

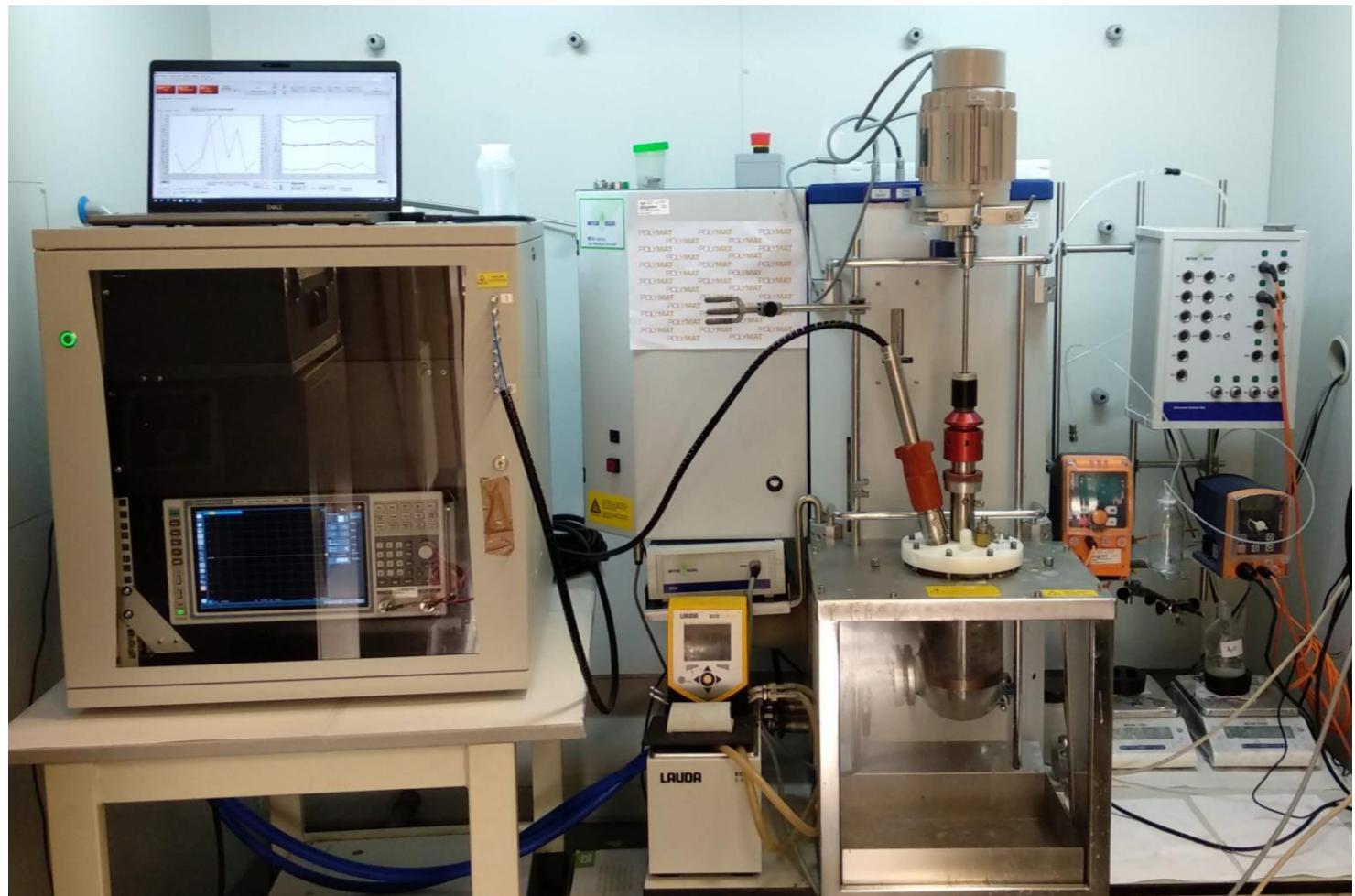




- Portable size
- High performance
- Adaptable to the process



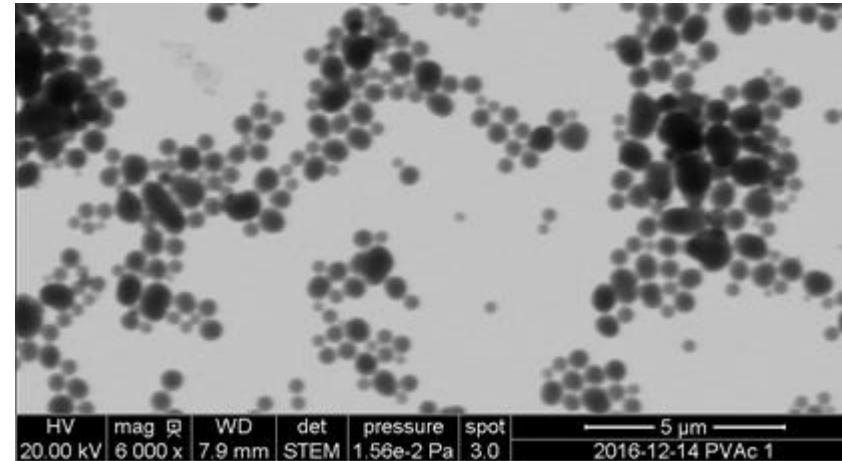
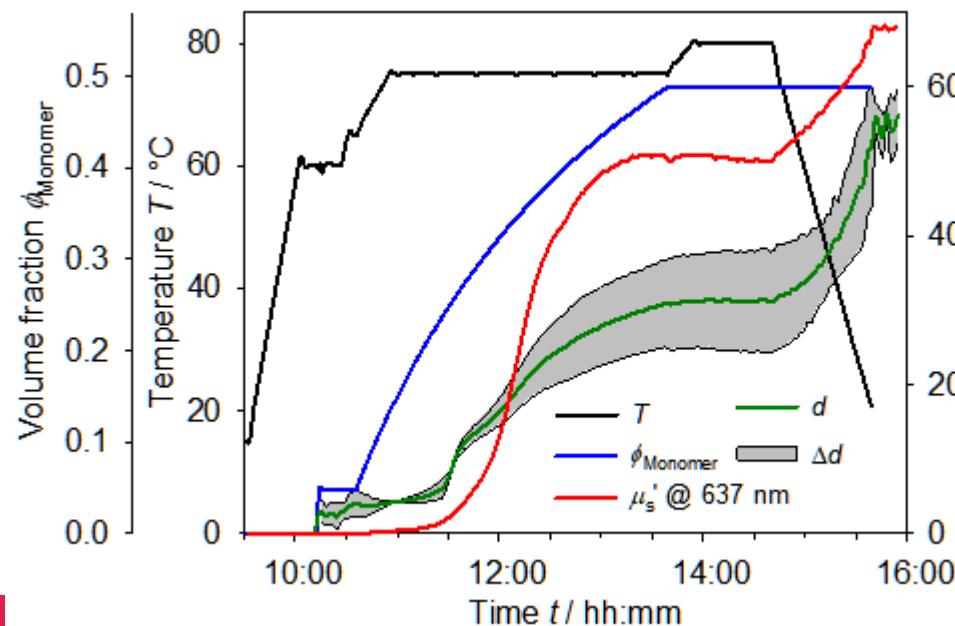
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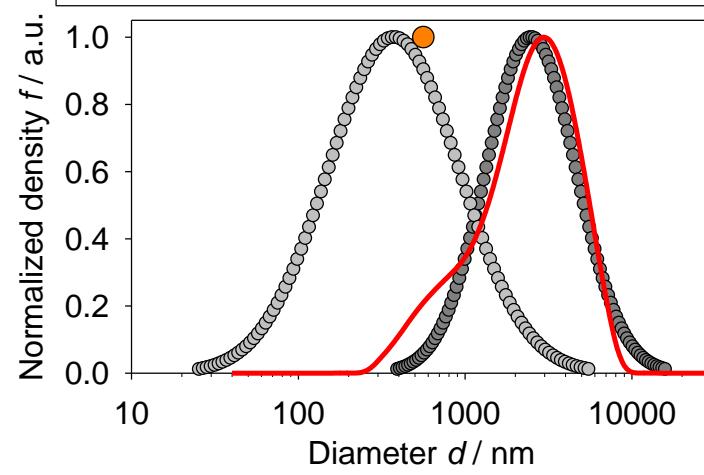
POLYMAT



Dr. D. Zehm, **Fraunhofer IAP**

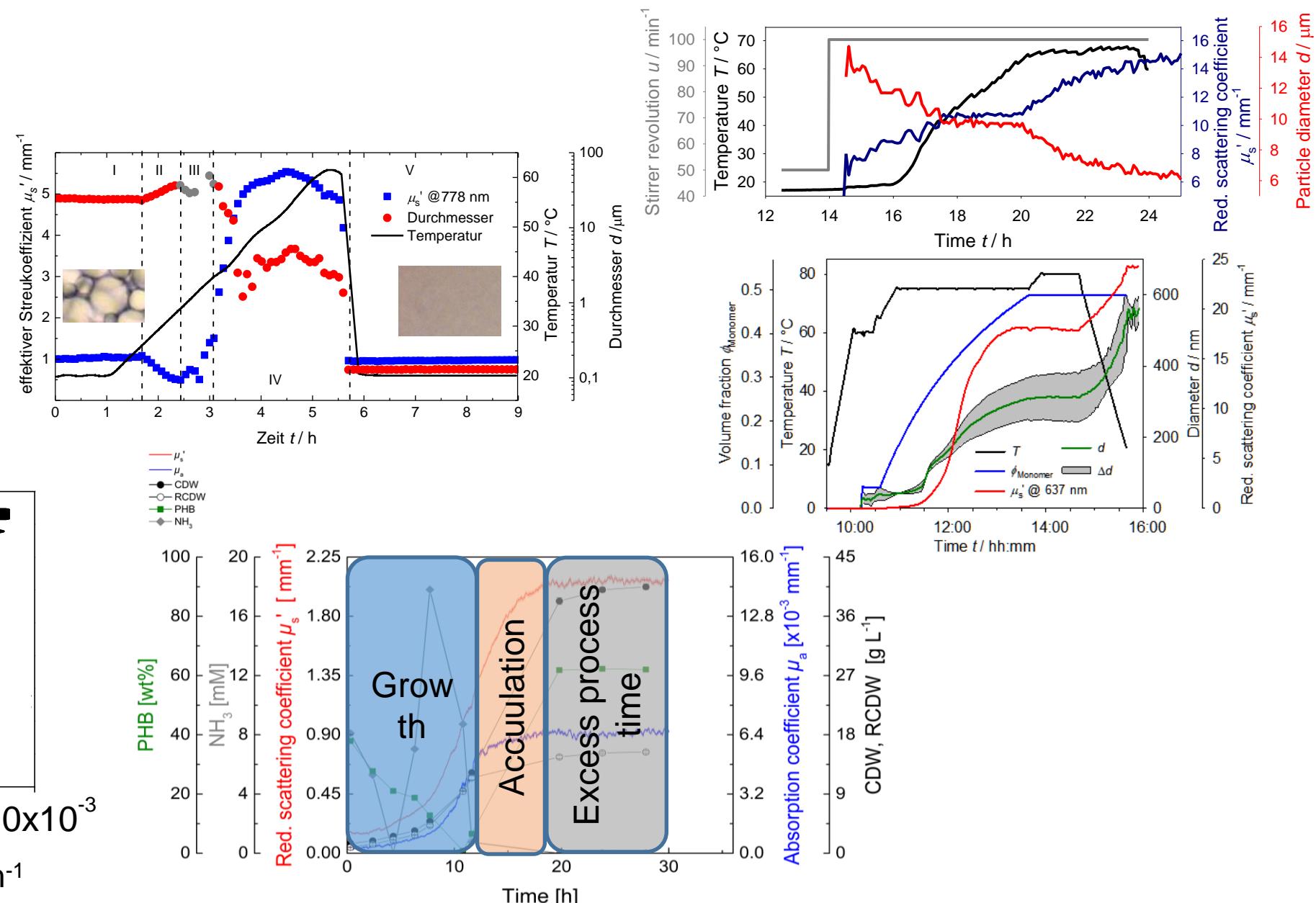
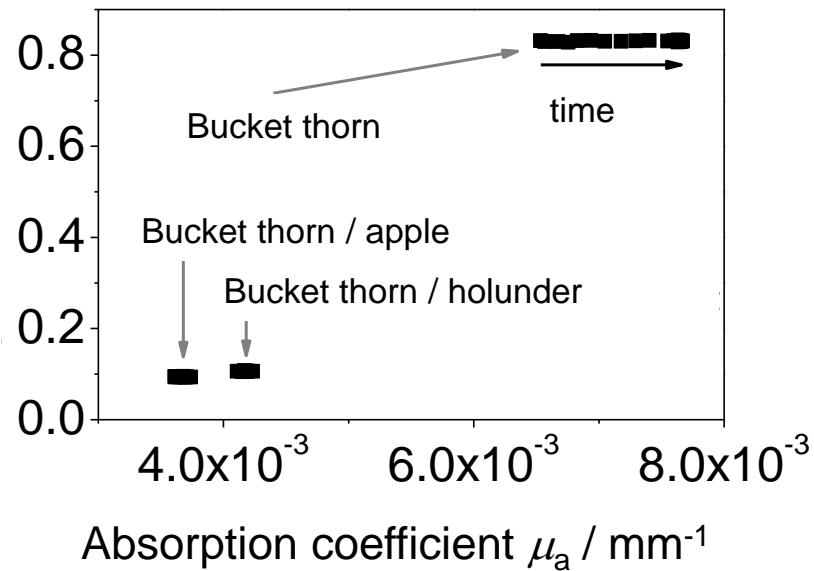


- volume based (by PDW)
- number based (by PDW)
- result from process measurement (by PDW)
- volume based (by SLS)



Application Examples

- Polymerization
- Emulsification
- Crystallization
- Fermentation
- Bioprocesses



Thank you!

NANOPAT: 




innoFSPEC
Innovative faseroptische Spektroskopie
und Sensorik

GEFÖRDERT VOM



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für Bildung
und Forschung

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Leibniz-Institut für
Astrophysik Potsdam



ZENTREN FÜR
INNOVATIONSKOMPETENZ
UNTERNEHMEN REGION
Die BMBF-Innovationsinitiative
Neue Länder



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Questions?

