Molecular and Biological Matter
"Nano-Science in Motion"

Frank Schreiber
http://www.soft-matter.uni-tuebingen.de

Molecular and Biological Matter "Nano-Science in Motion"

→ Was erwarte ich von meiner Bachelorarbeit ?

→ Welche Themen gibt es ?

→ Wie wähle ich „mein Thema" aus ?

→ Was sind die Kriterien zur Auswahl ?

→ Wie läuft die Arbeit in der Praxis ?

→ Was muss ich sonst noch wissen ?

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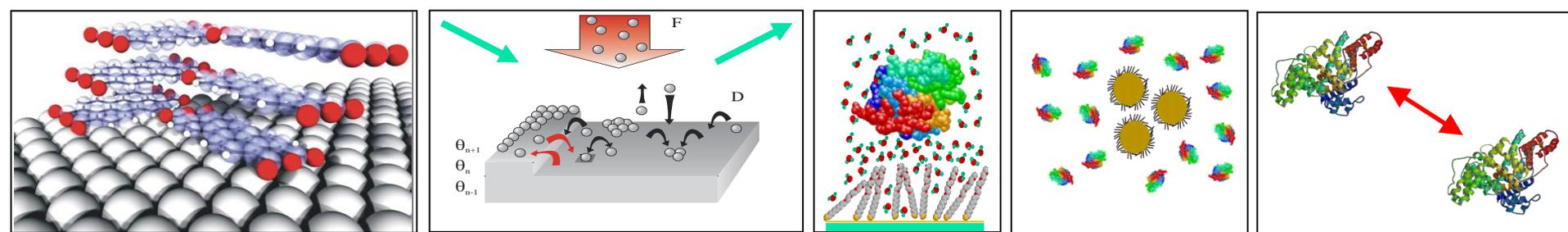
# Molecular and Biological Matter

Protein Biophysics: Bulk / Dynamics
(see also Fajun Zhang / see also collaboration with Grenoble)

Protein Biophysics: Interfaces


Organic and Hybrid Thin Films

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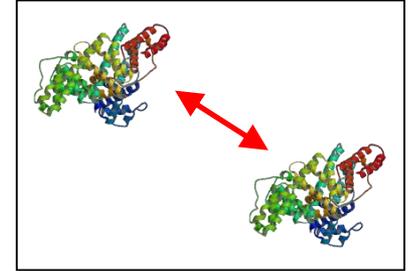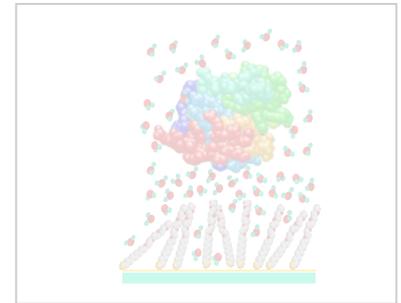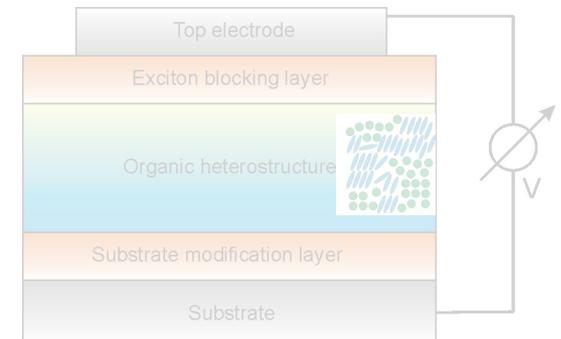
Protein Dynamics: Macroscopic Viscosity η

Viscosity η has to stay below threshold for injection !

Viscosity η

Diffusion D ~ 1 / η
(Stokes-Einstein)
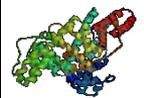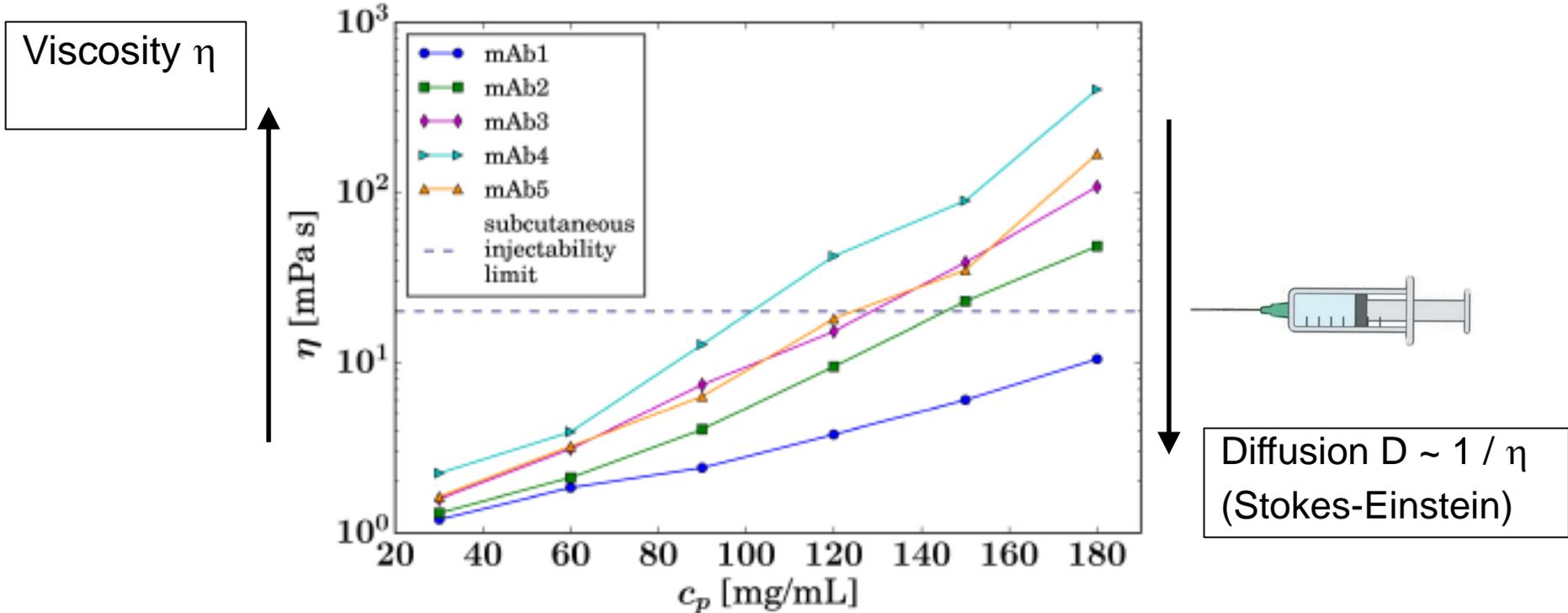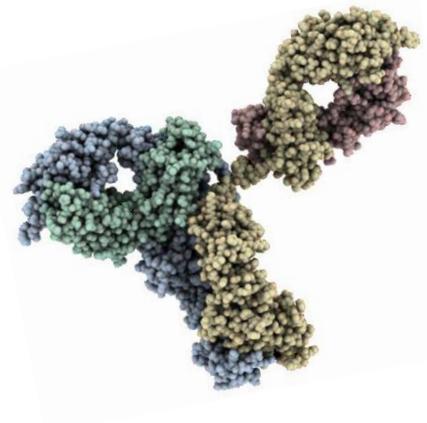
Protein Dynamics: Crowding

Now targeted deuteration of environment
→ Only proteins of interest visible
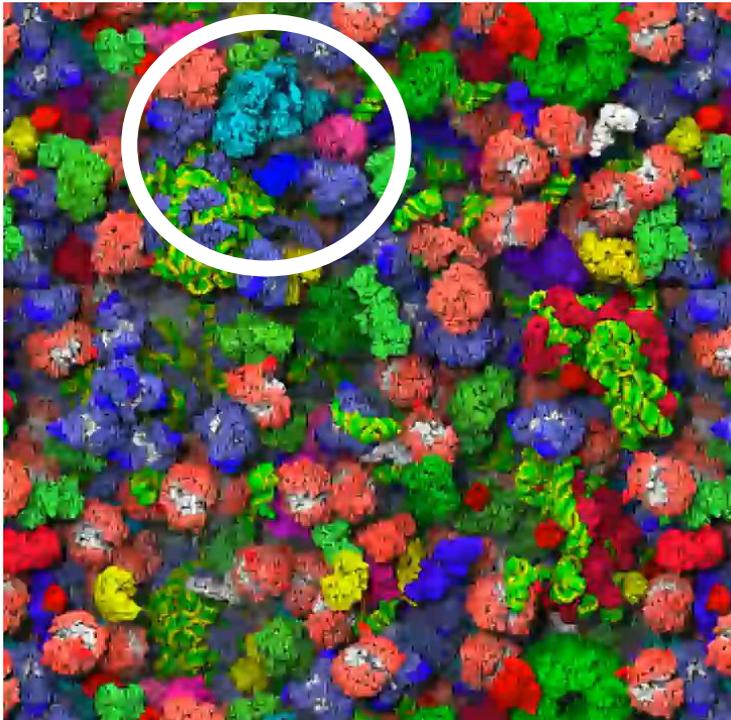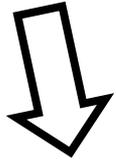
Self-diffusion probed by QENS
→ Hydrodynamic interactions important
   0.3 – 5.0 ns probed are short time diffusion
   no direct interactions
→ Slower for higher protein concentration

McGuffee & Elcock, Diffusion, Crowding & Protein Stability in a Dynamic Molecular Model of the Bacterial Cytoplasm. PLOS Computational Biology 6(3): e1000694 (2010)

F. Roosen-Runge et al., PNAS 108 (2011) 11815
M. Grimaldo et al., Quart. Rev. Biophys. 52 (2019), e7, 1
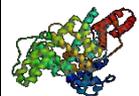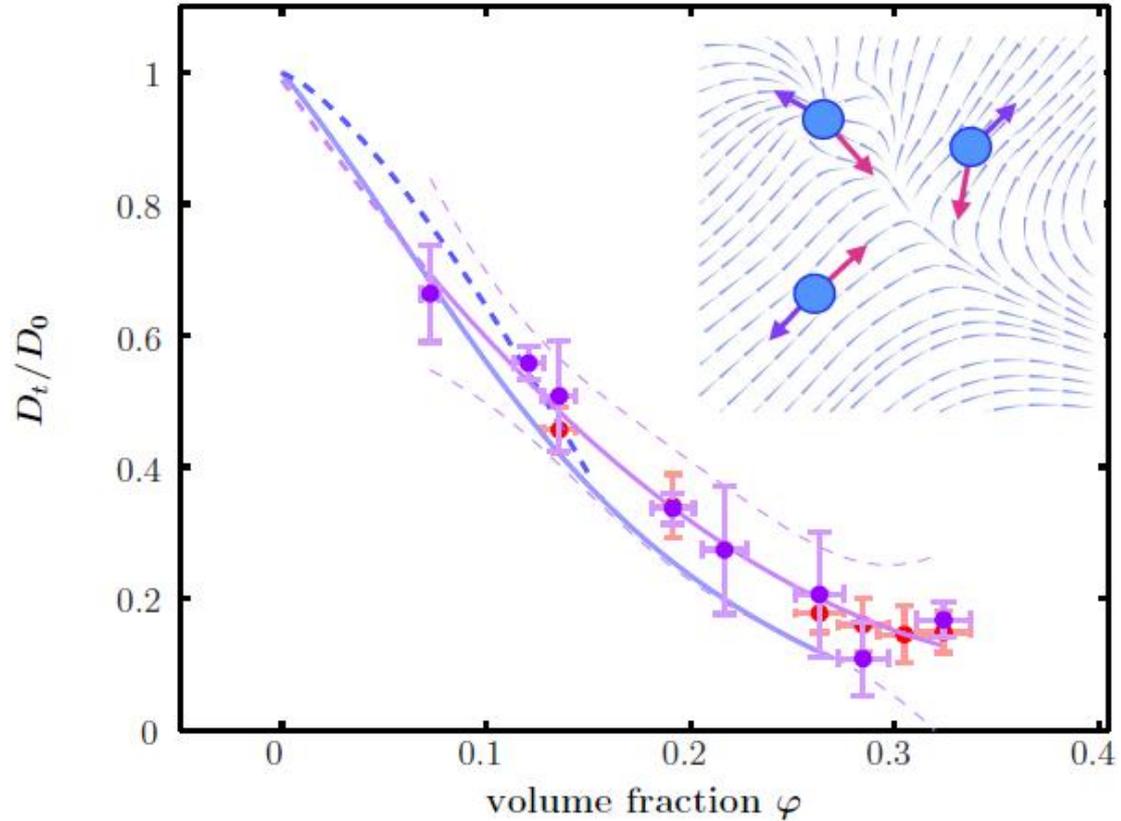
Protein Biophysics: Bulk / Dynamics

- Protein dynamics (rheology/scattering)
  … collaboration with Grenoble (ILL/PSCM)

# Molecular and Biological Matter
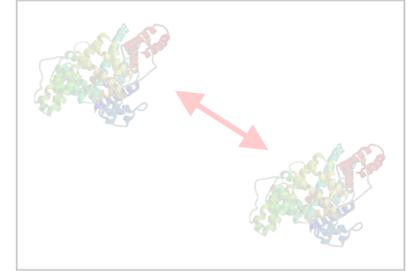
Protein Biophysics: Bulk
(see Fajun Zhang)

Protein Biophysics: Interfaces

Organic and Hybrid Thin Films

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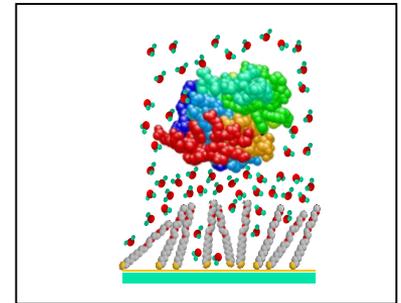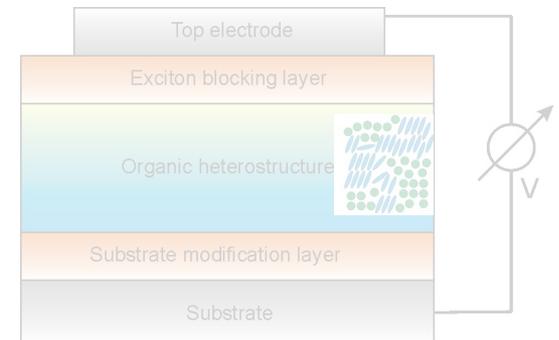
Protein Biophysics: Interfaces

Controlling protein-interface interactions ?
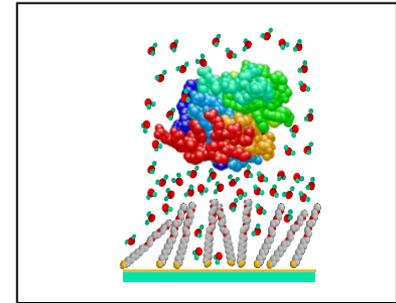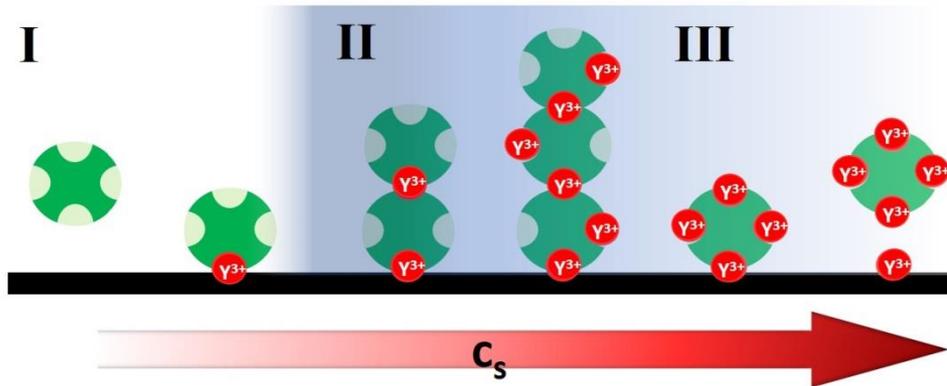
relevance for, e.g.
- biosensors, implants, stents ...
- biotechnology: biofouling, purification, ...
- structural biology: nucleation of crystals ...

# Protein Biophysics: Interfaces

Controlling protein-interface interactions ?
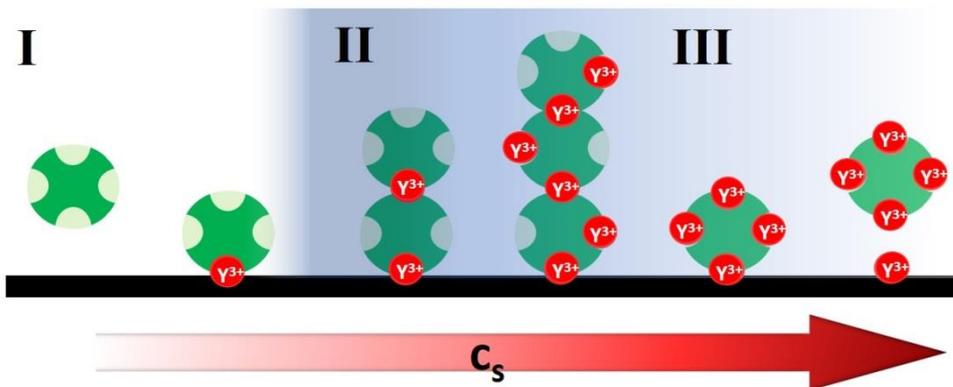
Interface adsorption
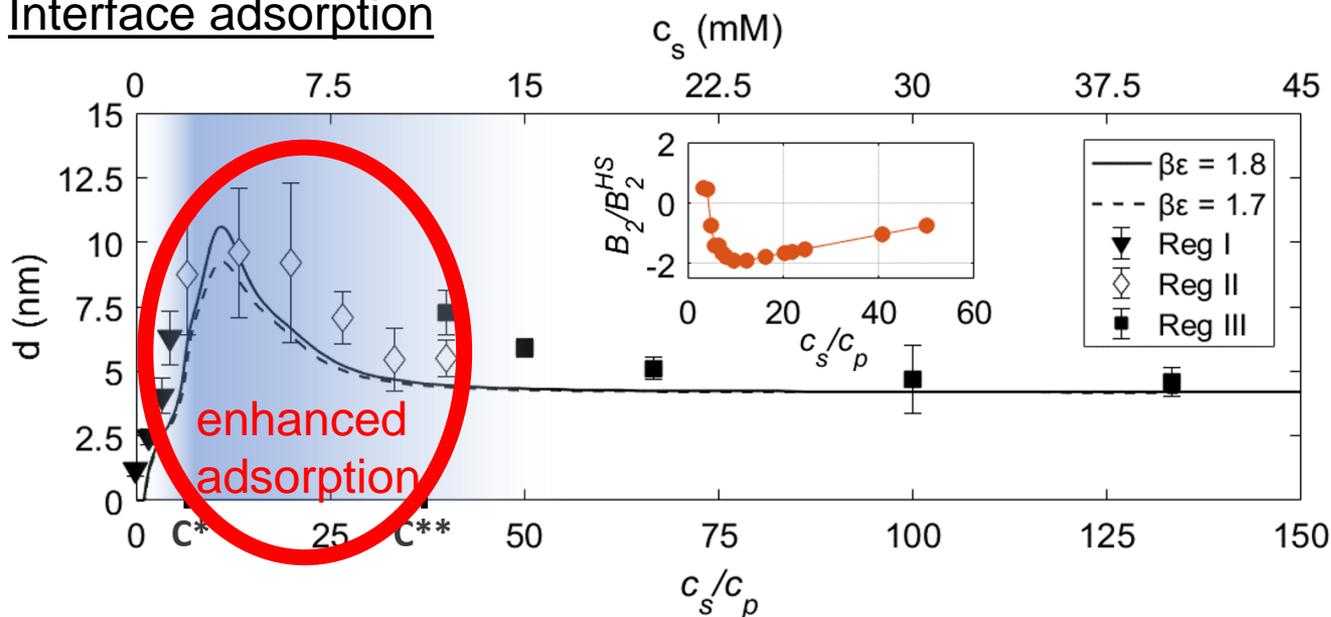
Phase diagram
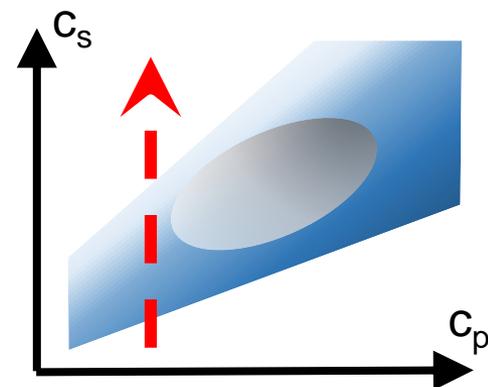
Protein Crystallisation induced by multivalent ions

100 µm
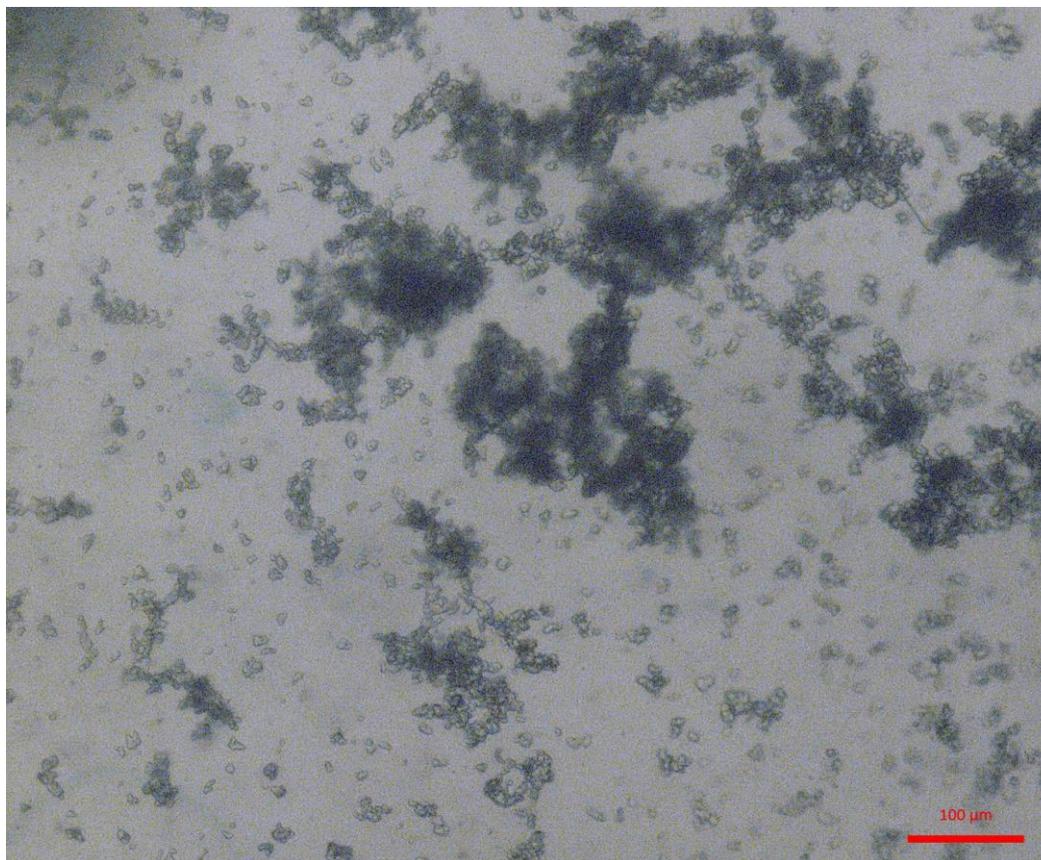
See also Cara Buchholz et al, J. Cryst. Growth 2022

Andrea Sauter et al, JACS 2015
Non-Trivial Nucleation of Protein Crystals in the Presence of Zn^{2+}

Protein Biophysics: Interfaces
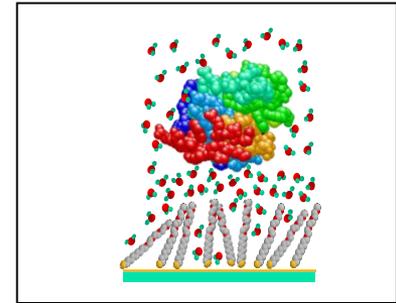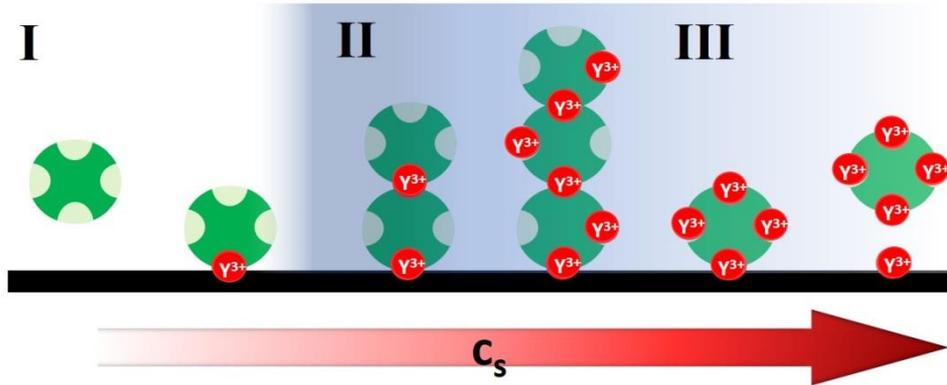
- Interface nucleation of protein crystals
- Tuning adsorption behavior
  a) Different salt ions
  b) Surface modifications through coatings
  c) Electrochemical potential
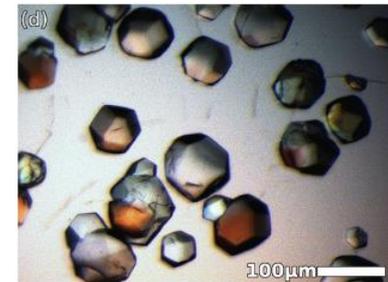
Molecular and Biological Matter
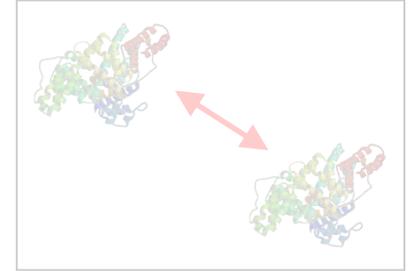
Protein Biophysics: Bulk
(see Fajun Zhang)

Protein Biophysics: Interfaces

Organic and Hybrid Thin Films

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Organic and Hybrid Thin Films

F

D

θ_{n+1}
θ_n
θ_{n-1}

| Top electrode |
| Exciton blocking layer |
| Organic heterostructure |
| Substrate modification layer |
| Substrate |

V

Samsung Galaxy with AMOLED display
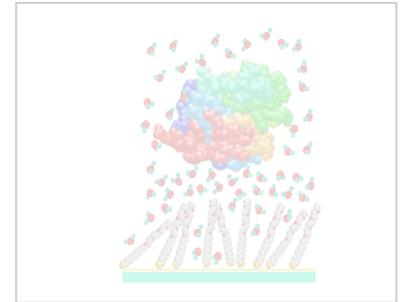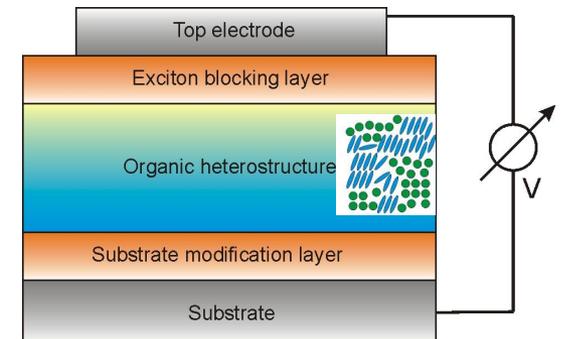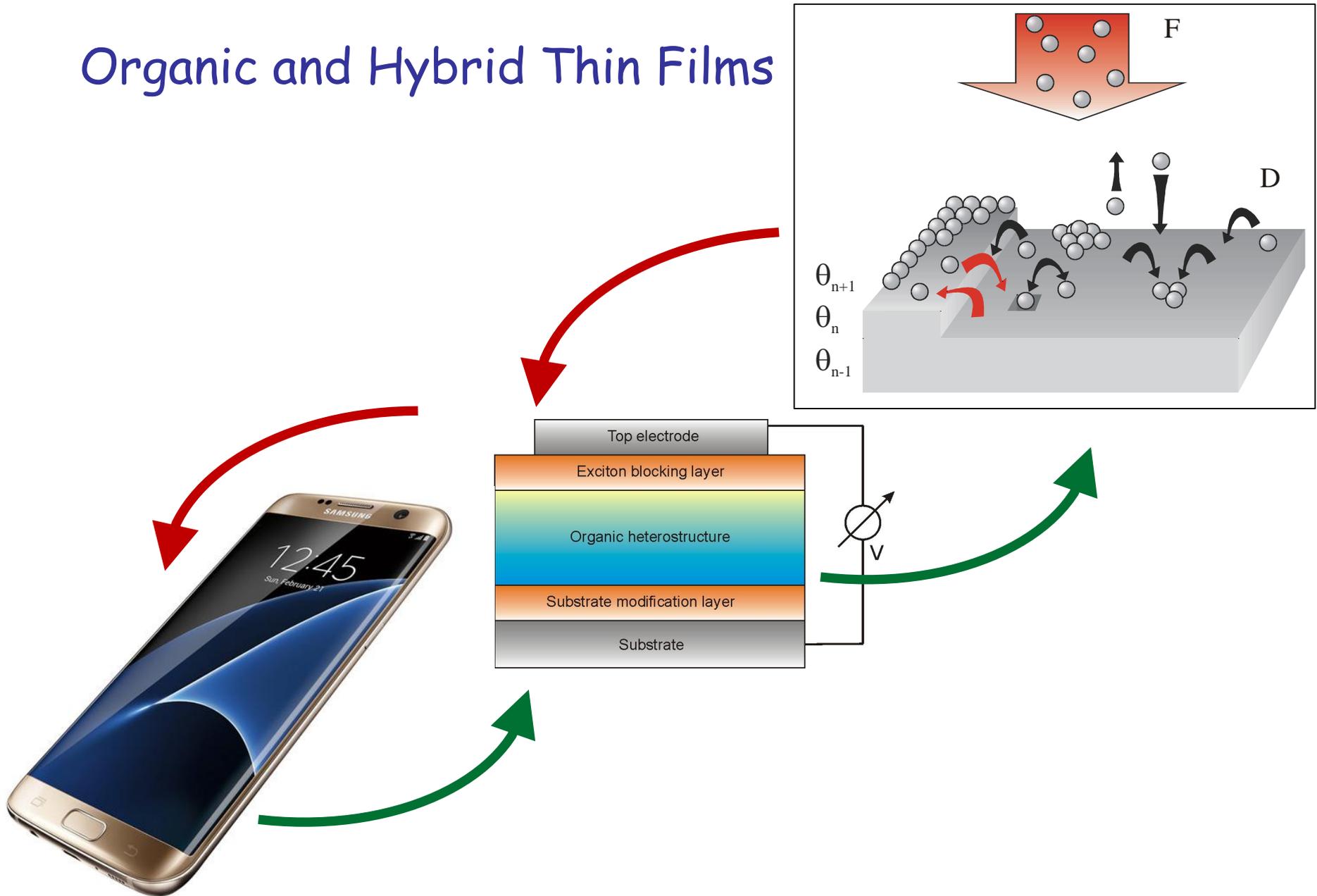
Organic and Hybrid Thin Films: Donor-Acceptor Structures

Similar concepts

→ for organic LEDs

→ for photovoltaics ("reverse LED")
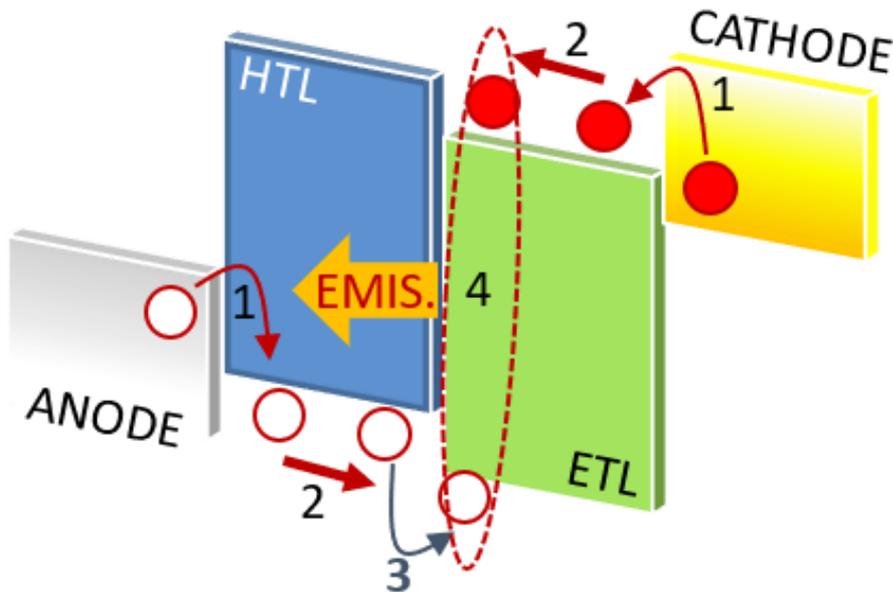
Planar Heterostructure (PHJ)
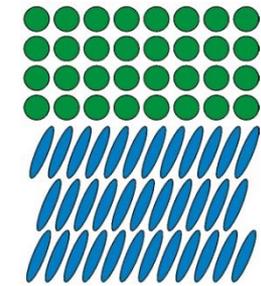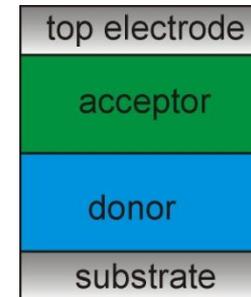
• high charge carrier mobility

• weak exciton dissociation

Mixed Heterostructure (BHJ)
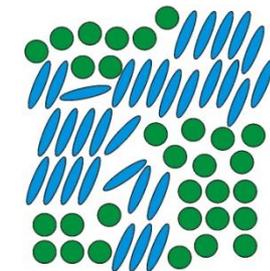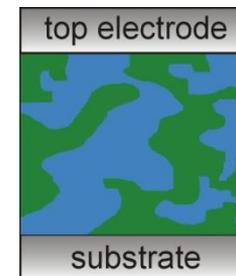
• low charge carrier mobility

• strong exciton dissociation

Internal Quantum Efficiency: $\eta_{IQE} = \eta_{A}\eta_{ED}\eta_{CT}\eta_{CC}$

Real-Time Growth
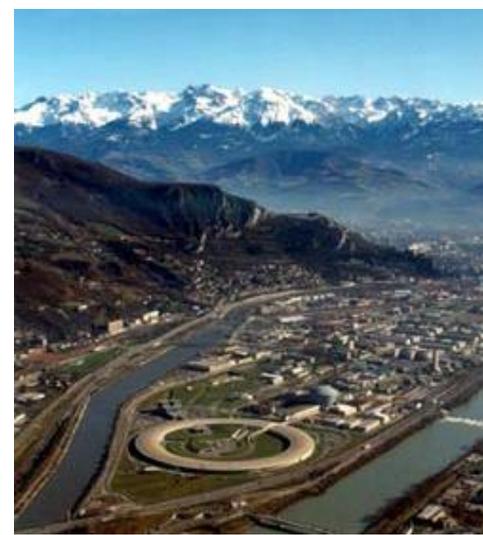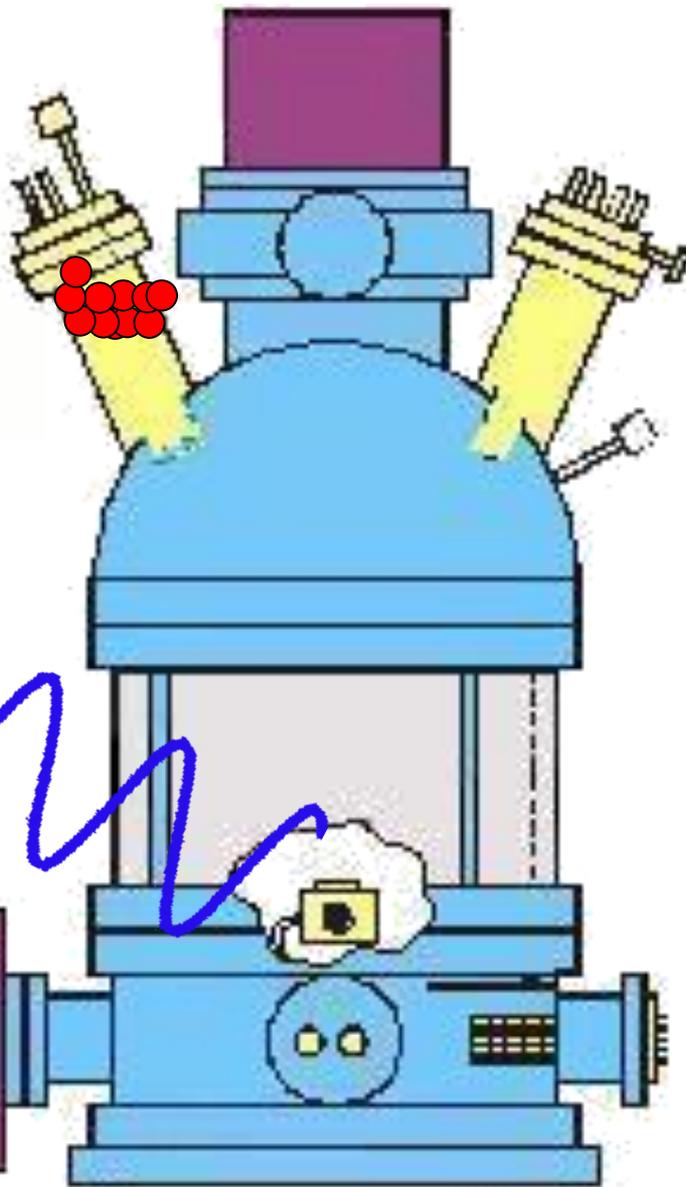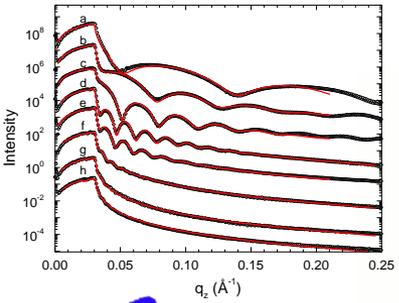
→ out-of-plane structure
→ in-plane structure

Growth data as I(q,t)

i.e. scanning the angles quickly

DIP on Si-oxide
growth at 130 deg. C
substrate temperature

Growth Rate 3 A / min
1 ML (standing up) is 16.5 A

Total growth time 100 min
Total thickness 300 A

0   10   19 Monolayers (standing up)

Charge Transfer Effects in Donor-Acceptor Mixtures
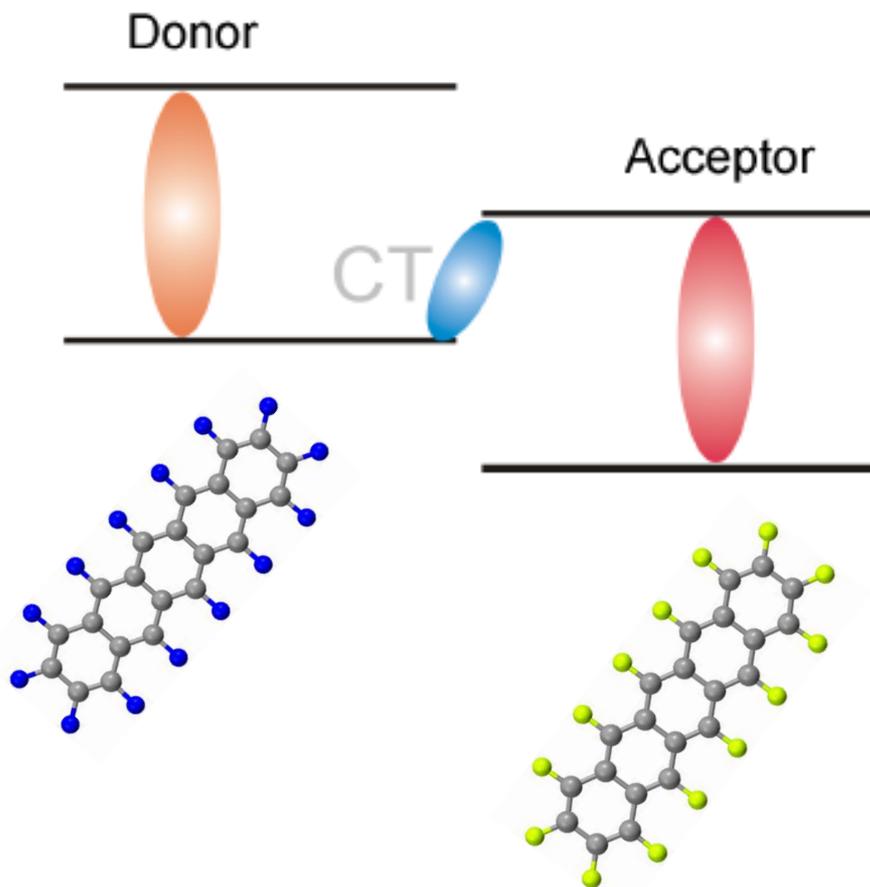
Optical Properties During Growth

using differential reflectance spectroscopy (DRS)
and spectroscopic ellipsometry with CCD detection

Zhang et al., PRL 104 (2010) 056601
Heinemeyer et al., PRL 104 (2010) 257401
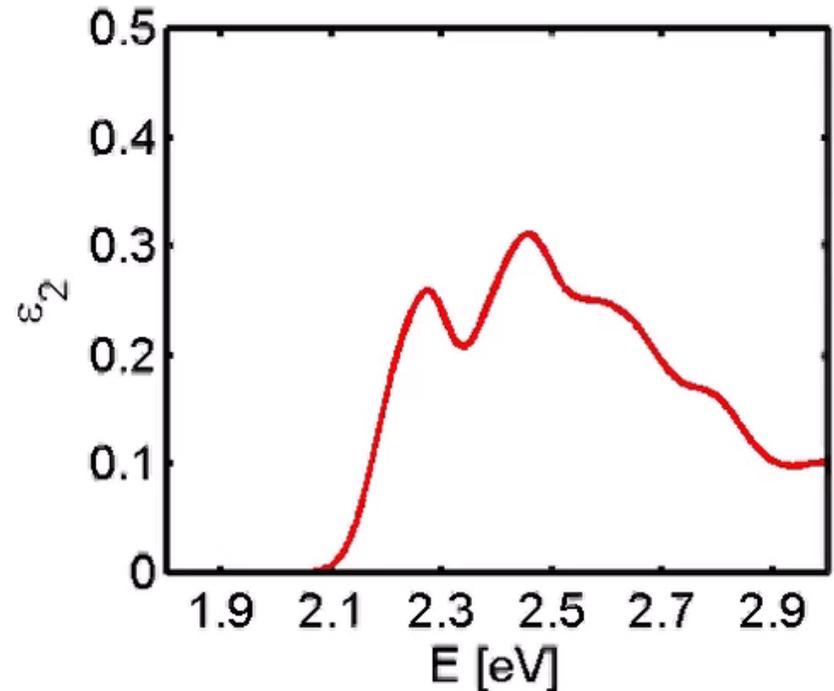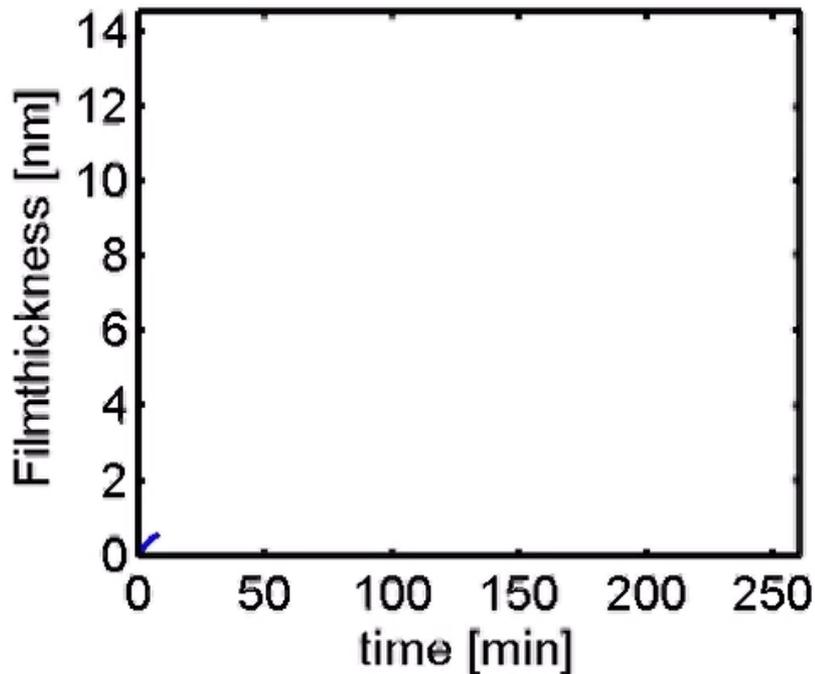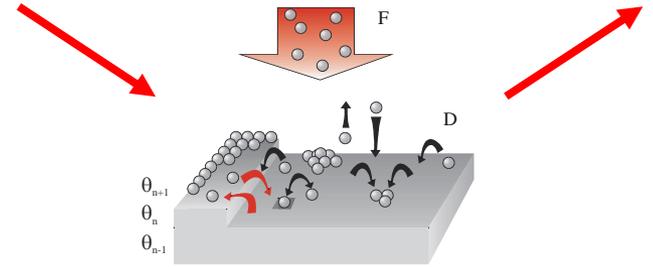
Organic and Hybrid Thin Films

- Photoluminescence of donor-acceptor mixtures
  as a function of temperature
- Hybrid materials (OSCs with Perovskites)
  optimization of spin coater for
  in-situ X-ray scattering

jeweils an Doktorand/in gekoppelt
jeweils max. 2 Kandidaten pro Thema
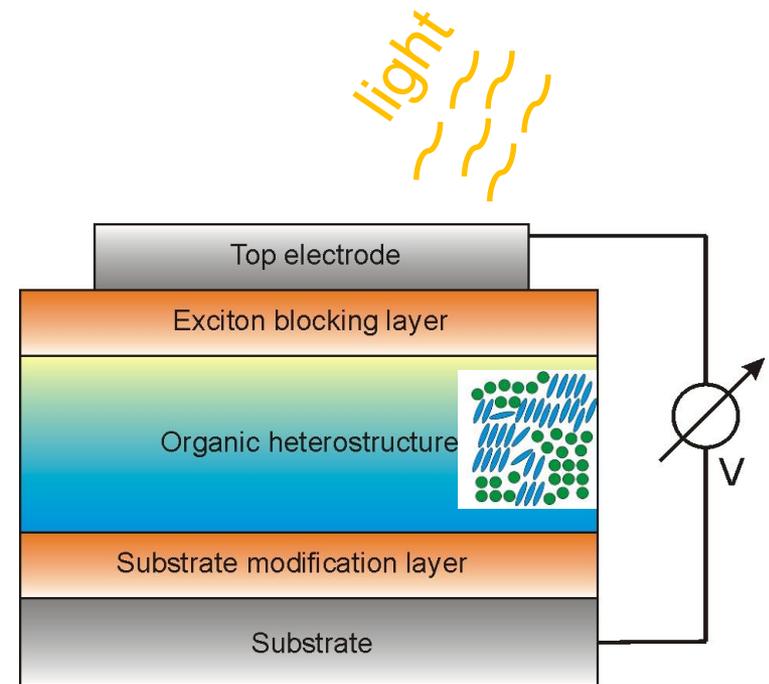
Protein Biophysics: Bulk / Dynamics

- Protein dynamics (rheology and scattering in Grenoble)

Protein Biophysics: Interfaces

- Interface nucleation of protein crystals
- Tuning adsorption behavior

Organic and Hybrid Thin Films

- Photoluminescence of donor-acceptor mixtures
- Hybrid materials (OSCs with Perovskites)

Machine Learning / Data Analysis

- ML for X-ray analysis of thin films

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