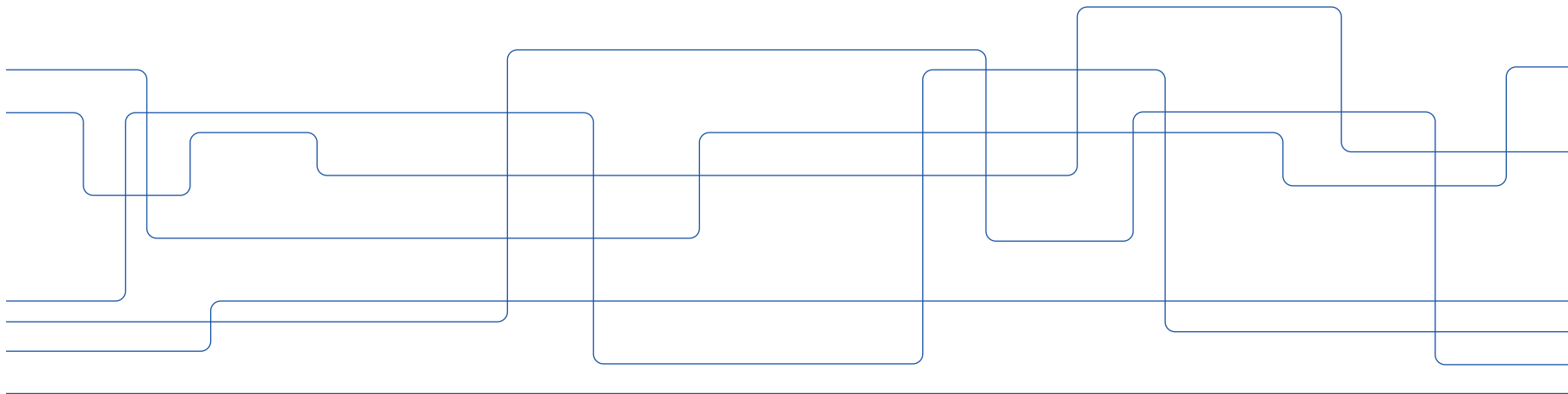




Water induced restructuring of organic electronics

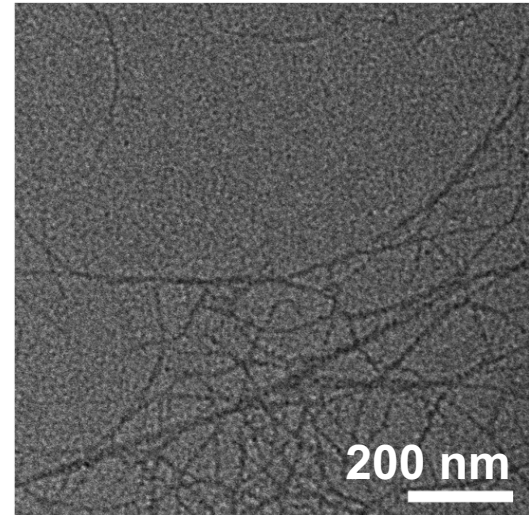
Calvin J. Brett

Swedish Neutron Week 2021 – GISANS session



Material selection

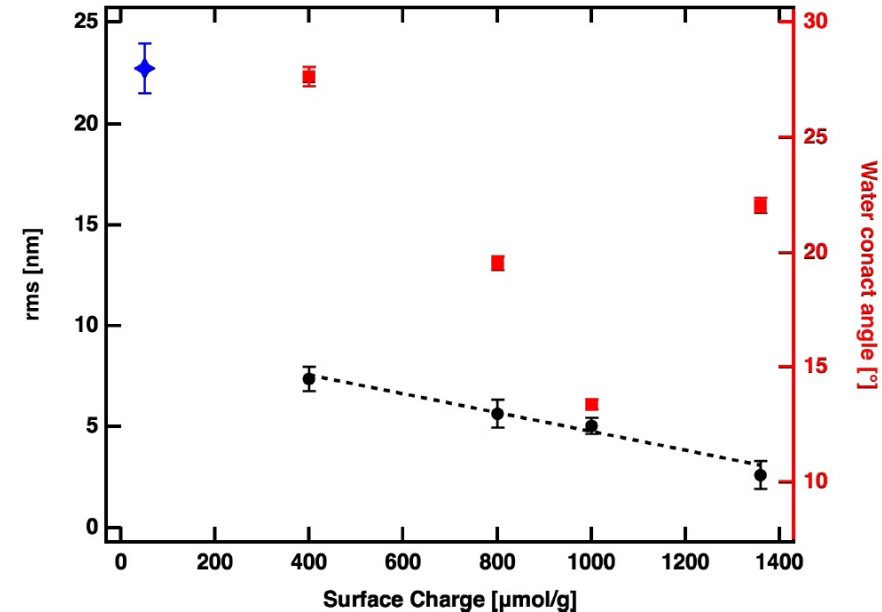
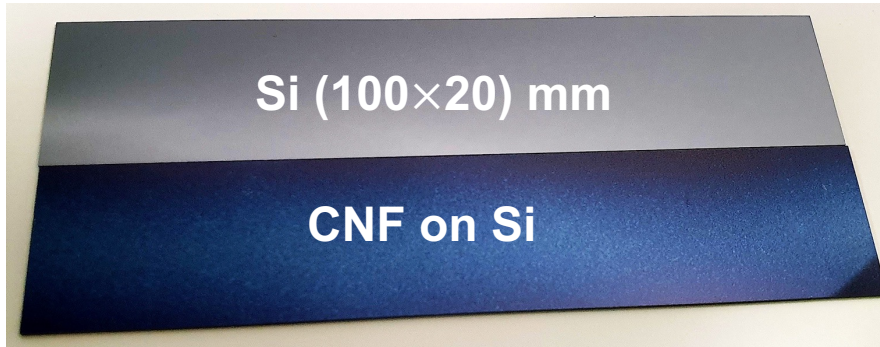
- Nanocellulose
 - Nanoscale
 - -Charged (carboxyl groups)
- PEDOT:PSS
 - Water soluble
 - Electric conductive



Brett *et al.*, Adv. Electron. Mater., 2100137 (2021)
Brett *et al.*, Macromolecules, 52, 12, 4721-4728 (2019)

CNF surface functionality

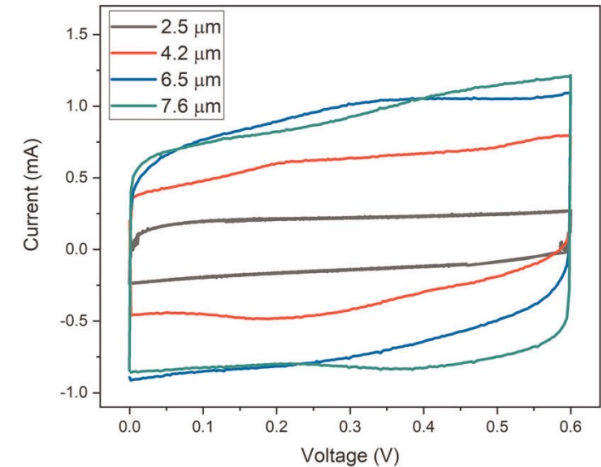
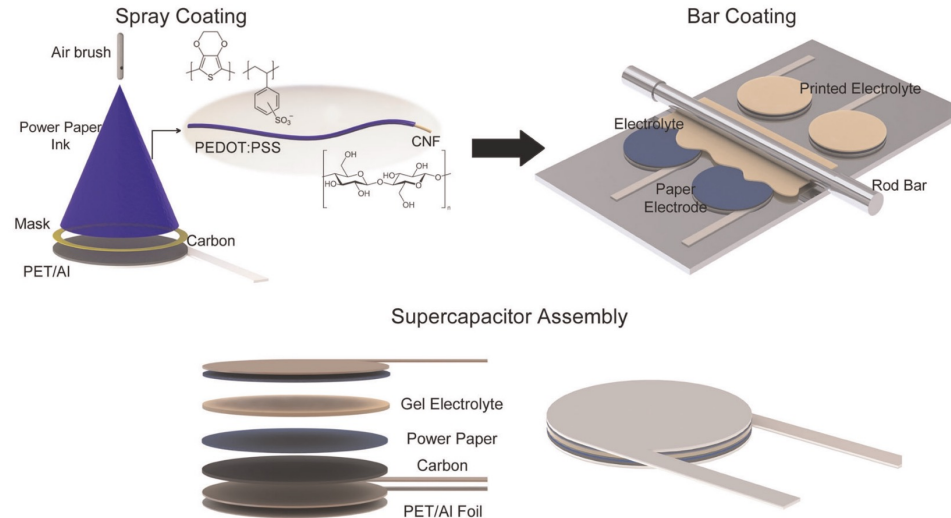
- Surface charge modification
- Decrease of roughness
- Change in wettability



Brett *et al.*, *Macromolecules*, 52, 12, 4721-4728 (2019)

PEDOT:PSS/CNF application

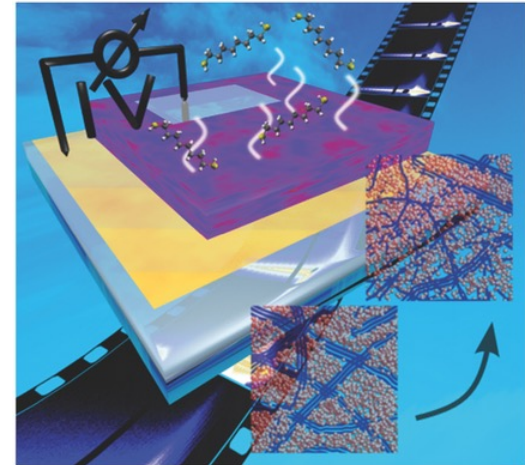
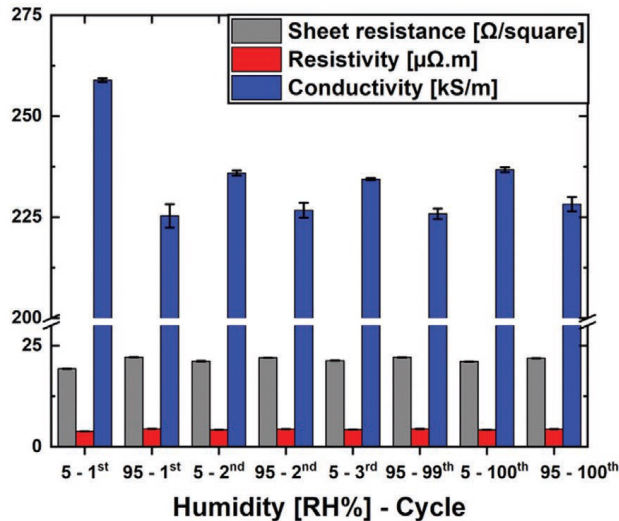
- Spray deposition of PEDOT:PSS/CNF
 - “Power paper”
- Electrode material
 - Eg. Super capacitors, OPVs



M. Say *et al.*, npj Flexible Electronics 4(1), 14 (2020)

Degradation of PEDOT:PSS/CNF electrode

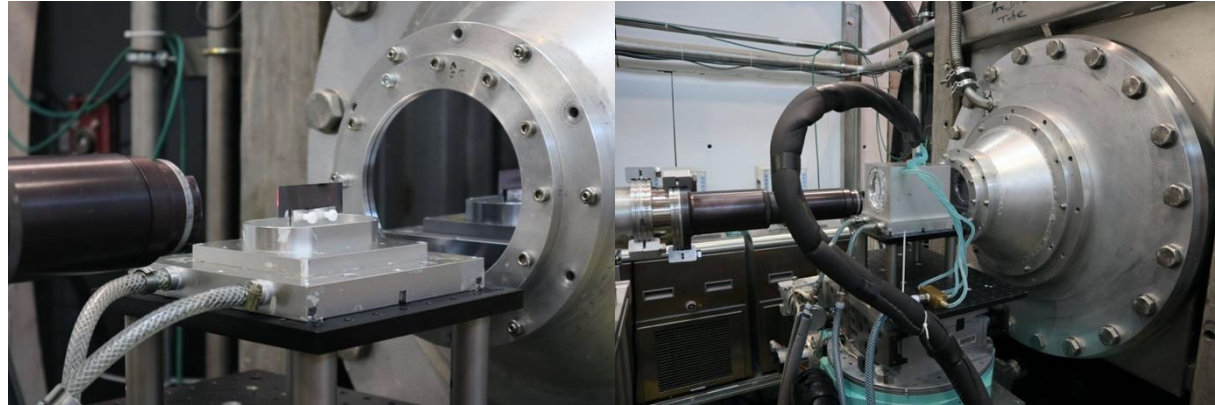
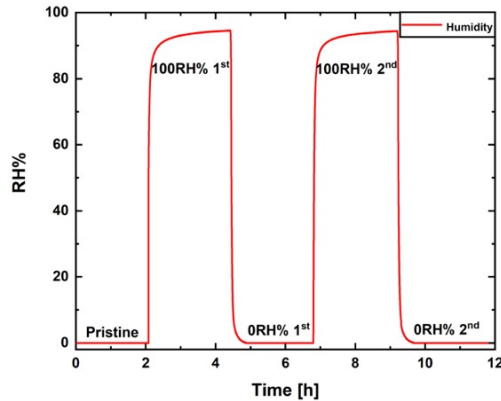
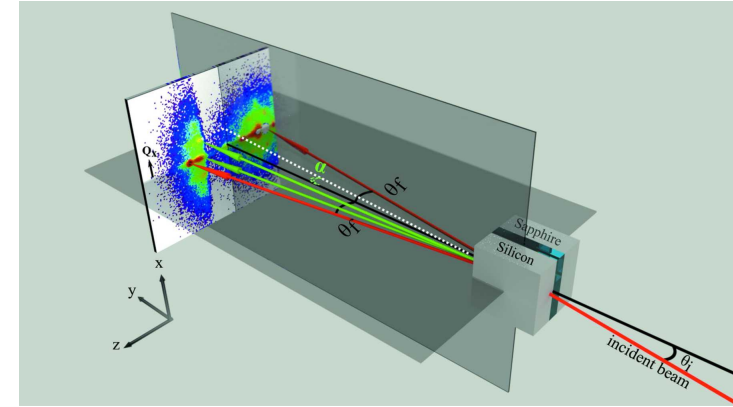
- Physical degradation of conductivity
 - Water vapor
- Implicated by restructuring of the composite?
- Similar effects are seen in OPVs during operation



Brett *et al.*, Adv. Electron. Mater., 2100137 (2021)
 Schaffer *et al.*, Adv. Energy Mater., 6, 1600712 (2016)

GISANS humidity study

- Experiment at D22 @ ILL
- Humidity chamber (TUM, Munich)
- GISANS at $\theta_i = 1^\circ$

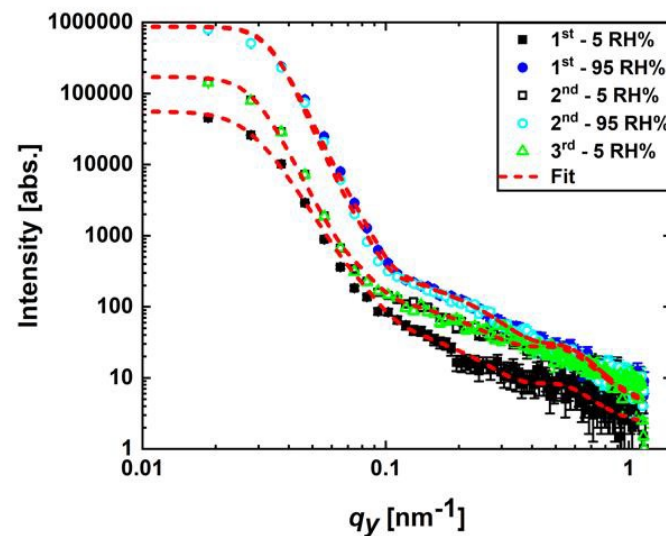
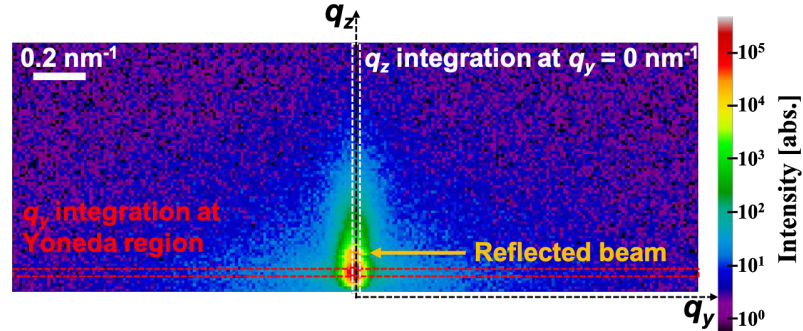
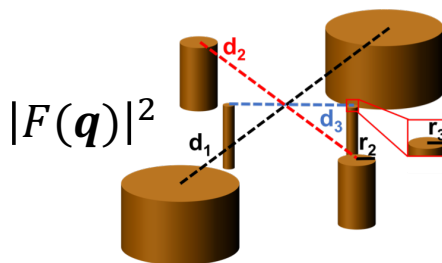
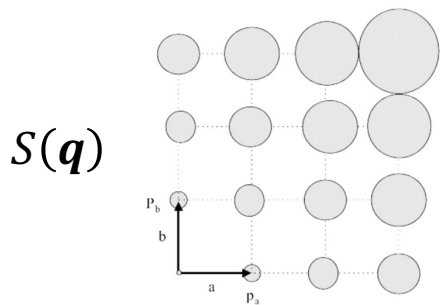


Brett *et al.*, Adv. Electron. Mater., 2100137 (2021)

S. Nouhi et al., J. Appl. Crystallogr., 50, 1066-1074 (2017)

GISANS experiment

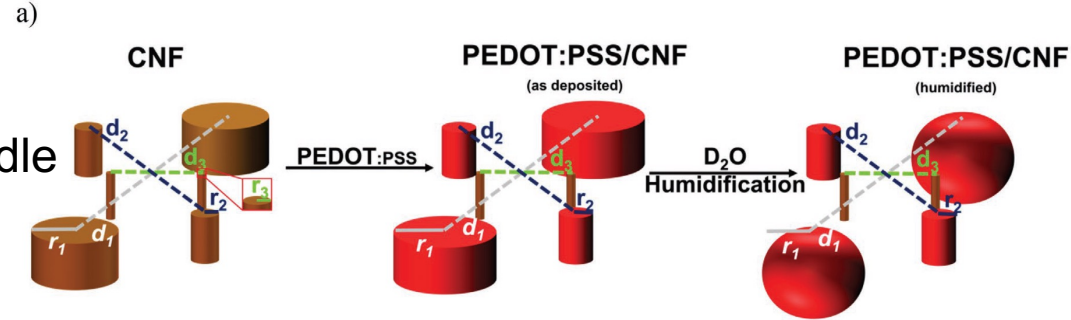
- q_z : In-plane
 - nano particle height, roughness
- q_y : Out-of-plane
 - distances, radii
- Scattered intensity (+ DWBA): $I(\mathbf{q}) = \langle |F(\mathbf{q})|^2 \rangle \cdot S(\mathbf{q})$
- Structure factor $S(\mathbf{q}) \rightarrow$ Paracrystal
- Form factor $|F(\mathbf{q})|^2$
 - Cylindrical / spherical model



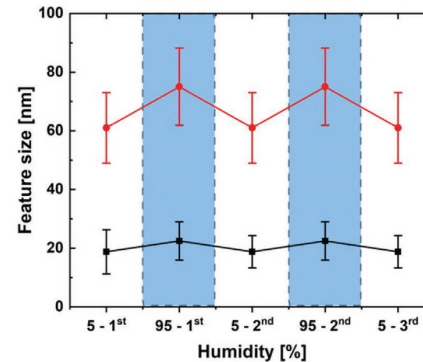
Brett *et al.*, Adv. Electron. Mater., 2100137 (2021)
 R. Lazzari, J. Appl. Crystallogr., 35, 406-421 (2002)

GISANS experiment

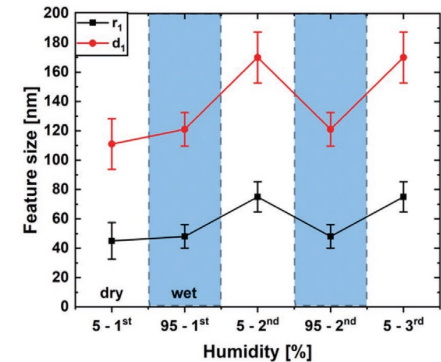
- Modelled analysis
- 3 modal features
- Smallest feature CNF bundle
- Change of large features



b)



c)



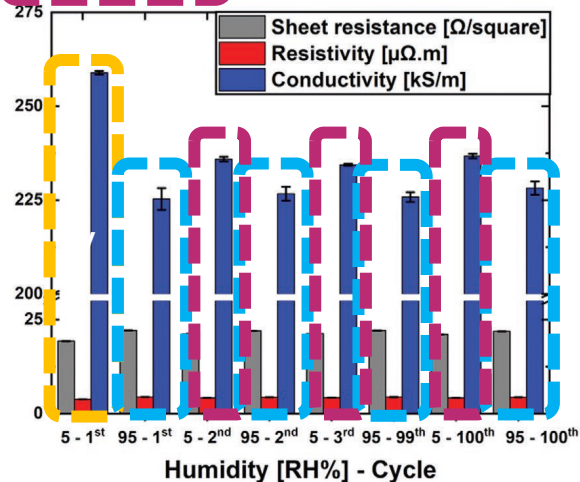
Brett *et al.*, Adv. Electron. Mater., 2100137 (2021)

3 Phase model

I as deposited

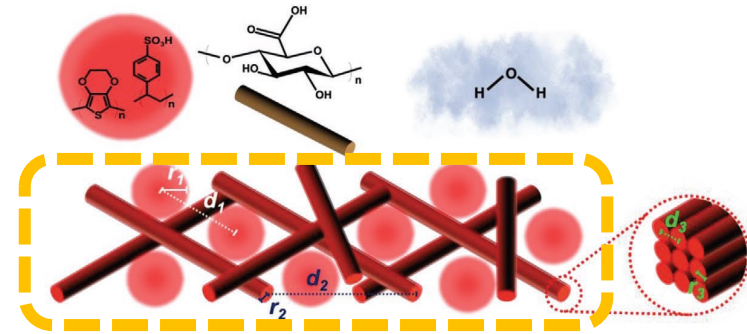
II humid environment

III redried

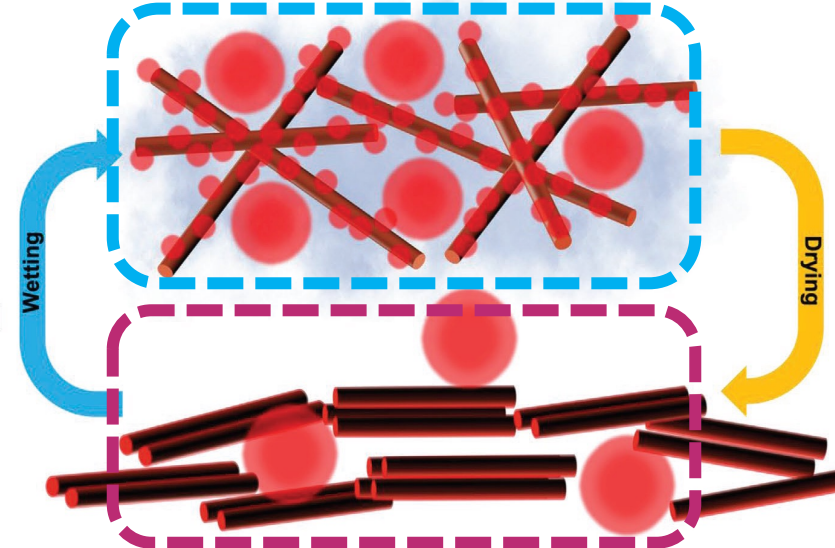


Brett *et al.*, Adv. Electron. Mater., 2100137 (2021)

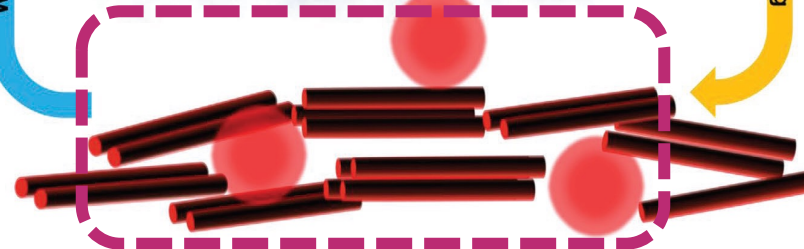
I



II

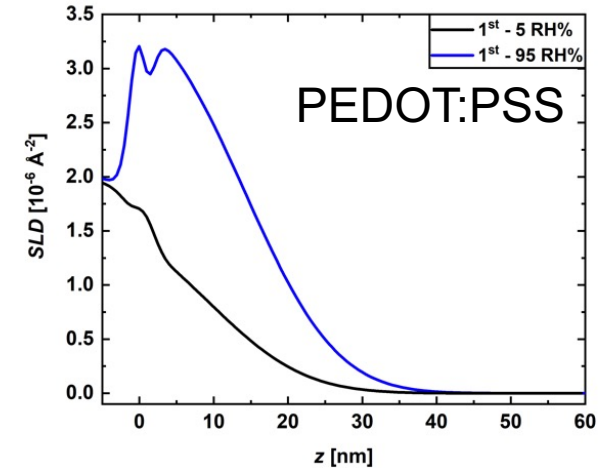
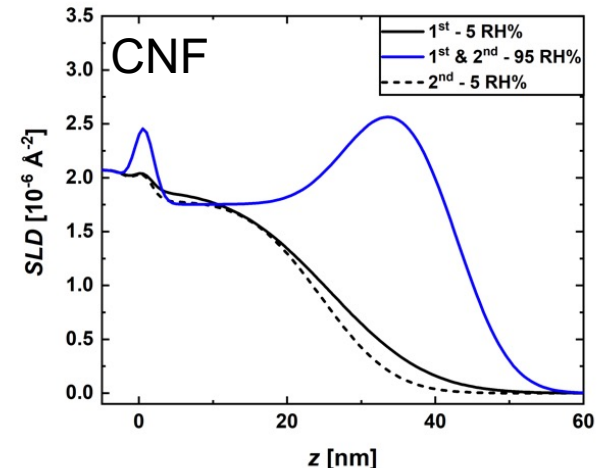
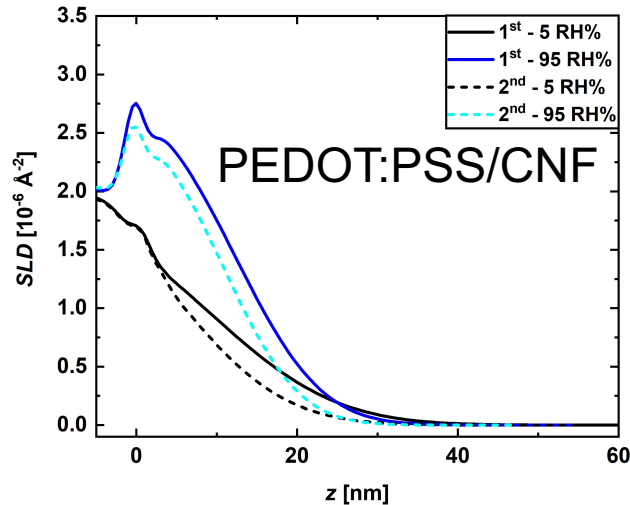


III



TOF-NR

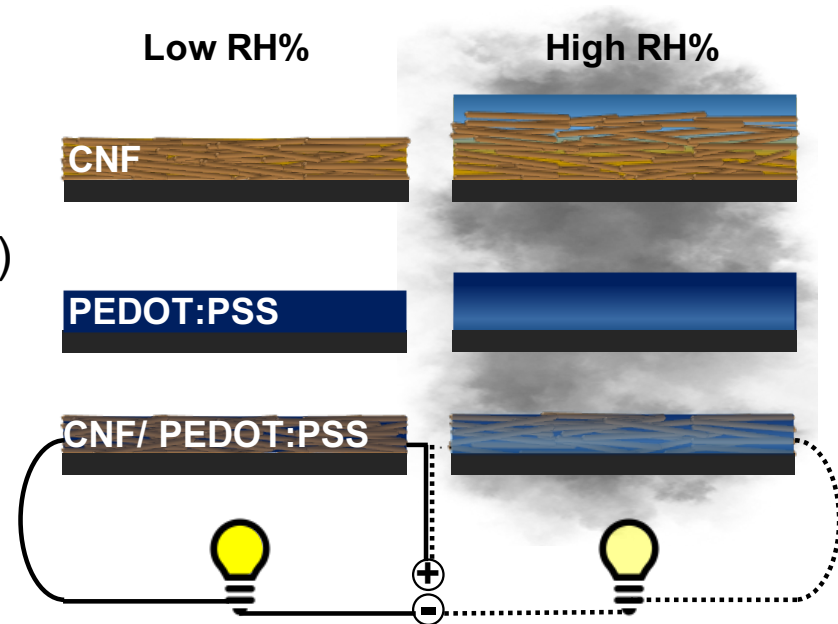
- SOFIA @ J-Parc
- Swelling of components / composite
- Water layer on top of CNF
- Water penetrates the full PEDOT:PSS layer
- Swelling prevented in composite



Brett *et al.*, Adv. Electron. Mater., 2100137 (2021)

Conclusion

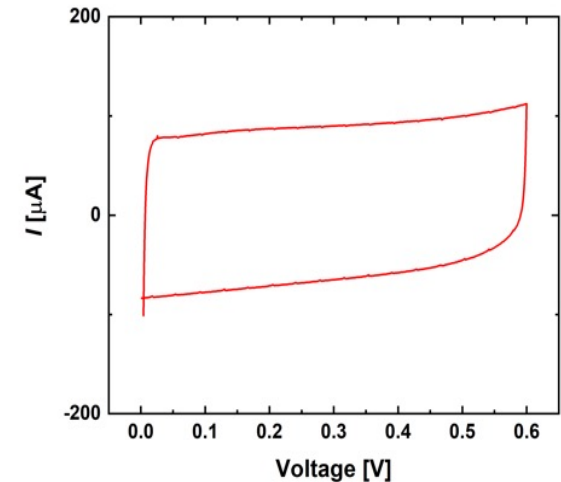
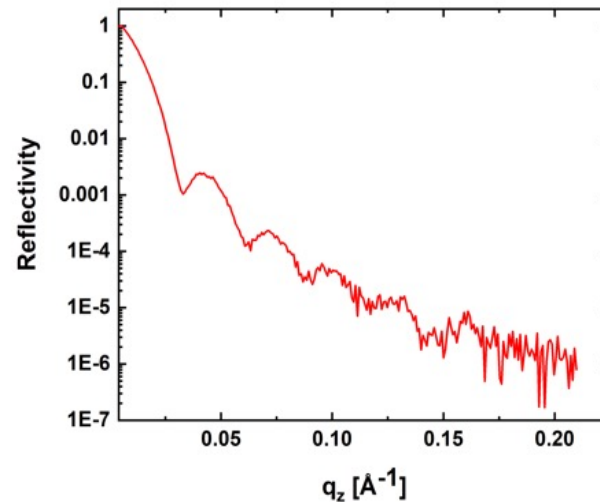
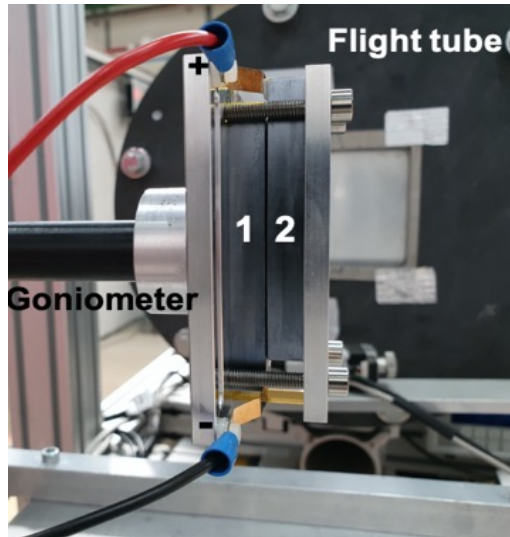
- Electrical conductivity
 - Initial decrease
 - Cyclic
- Reorientation of PEDOT:PSS/CNF
 - Cyclic
- Equilibrium states (1. wet/ 2. redried)
- Composite prevents swelling
 - Reinforcing effects



Brett *et al.*, Adv. Electron. Mater., 2100137 (2021)

Outlook

- *In situ in operando* study of super cap. @SuperADAM (w. Alexei Vorobiev)
 - In progress





Team & Collaboration



Stephan V. Roth



Lionel Porcar

Ola K. Forslund
Elisabetta Nocerino
Nami Matsubara
Martin Månsson
L. Daniel Söderberg



Norifumi L. Yamada



Lucas P. Kreuzer
Tobias Widmann
Peter Müller-Buschbaum

Strategy Fund DSF
Supporting strategic cooperation at DESY