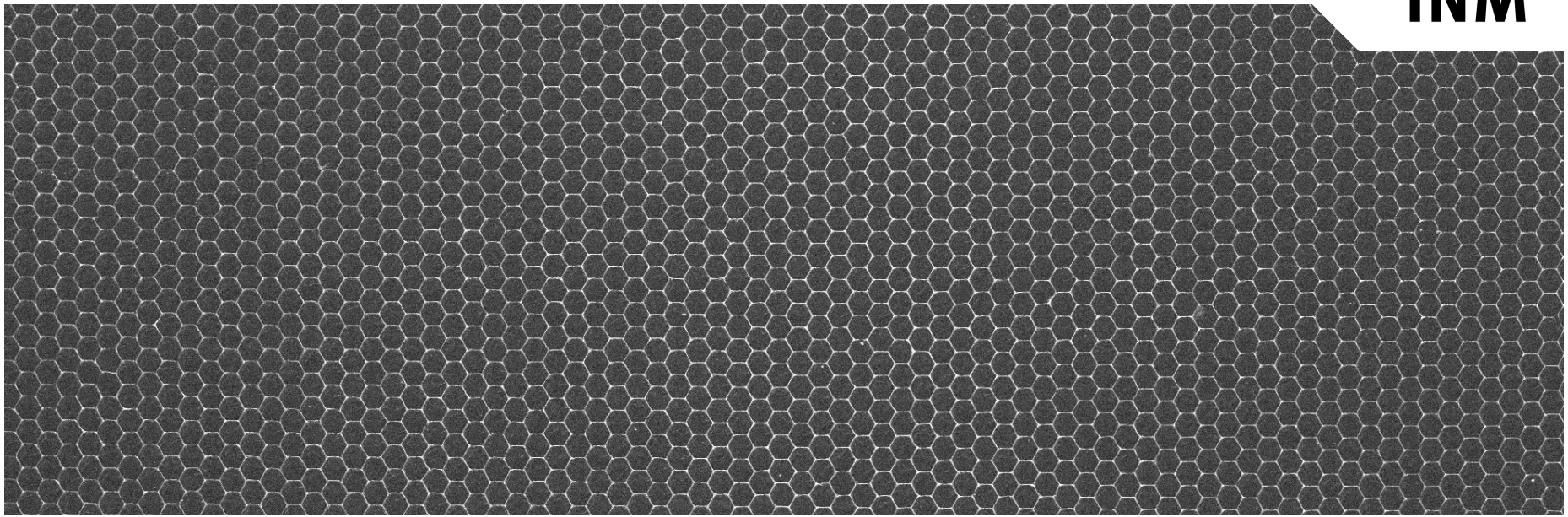
New Thinking. New Materials.

INM

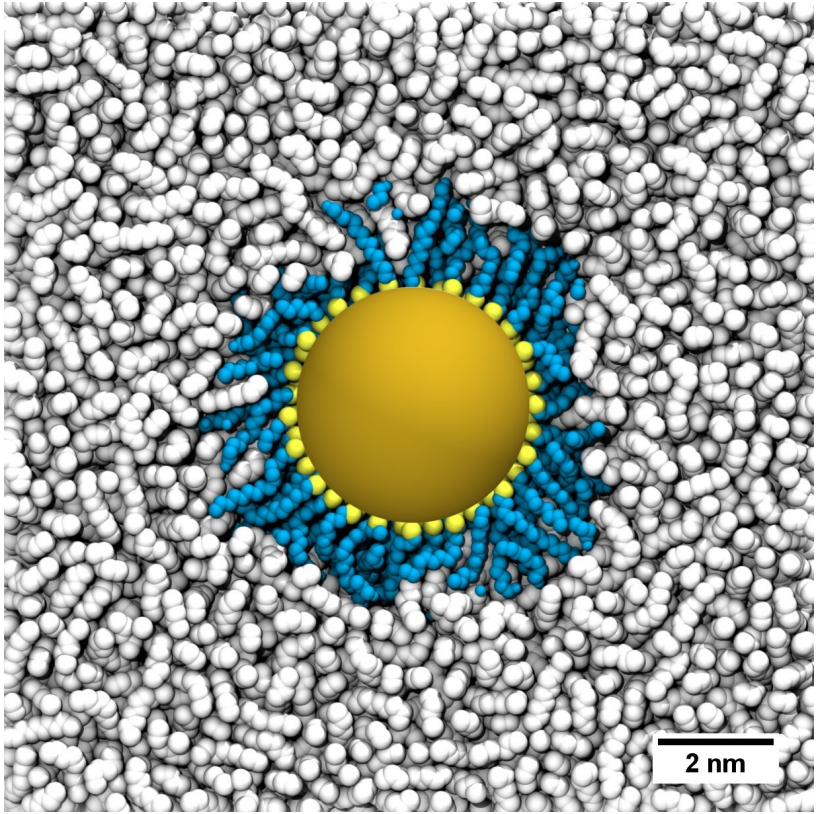


Self-assembling ultrathin nanowires into bundles, fibres, and transparent electrodes

Beate Reiser, Simon Bettscheider, Lukas Engel, and Tobias Kraus

INM – Leibniz-Institute for New Materials and Saarland University, Saarbrücken, Germany

Introduction: apolar nanoscale colloids



Inorganic nanoparticles with apolar shells:

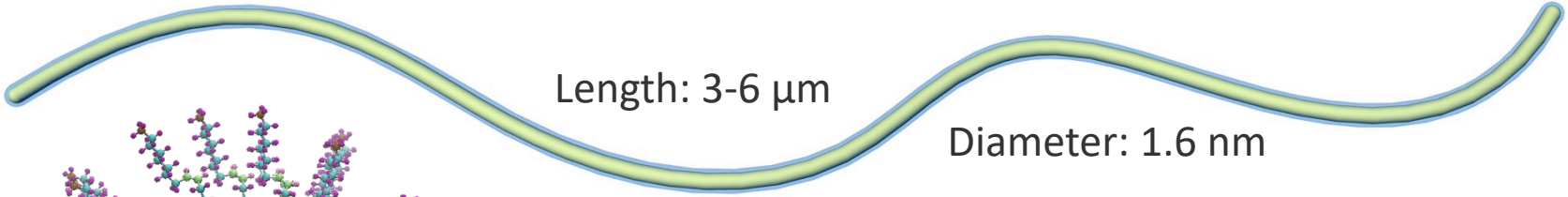
- Soft spheres, often attractive $O(k_BT)$
- Molecular configurations affect interactions
- Small changes affect colloidal stability
- Geometries and properties of agglomerates sensitively depend on conditions

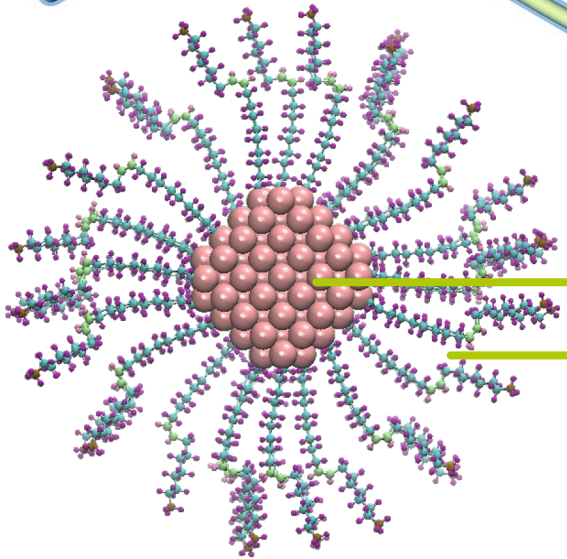
Relevant for commercially important particles.

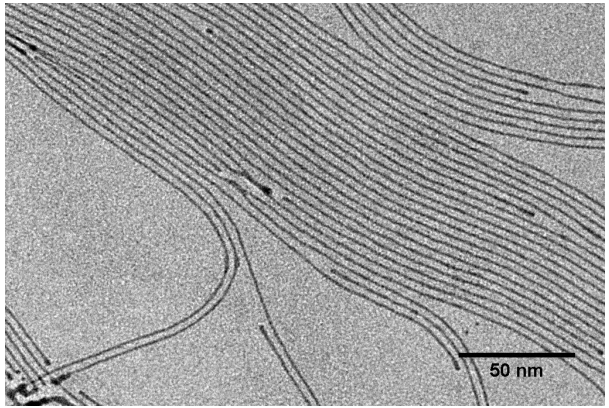
Simulation of a hexadecane-covered particle in hexane:

Dr. Asaph Widmer-Cooper and Debora Monego,
University of Sydney, Australia

Introduction: apolar nanoscale colloids



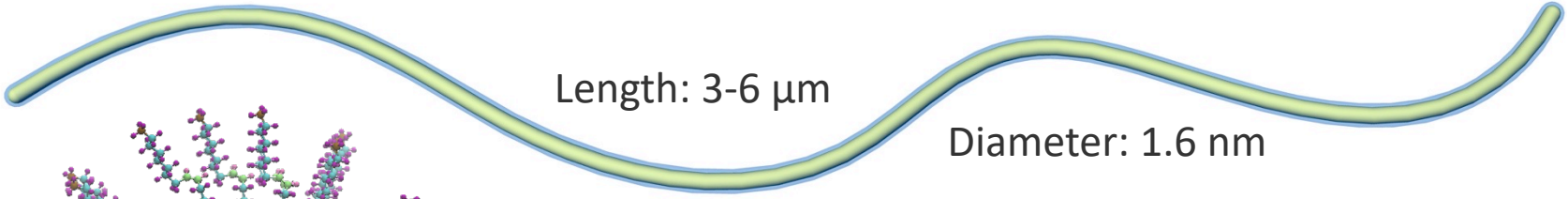


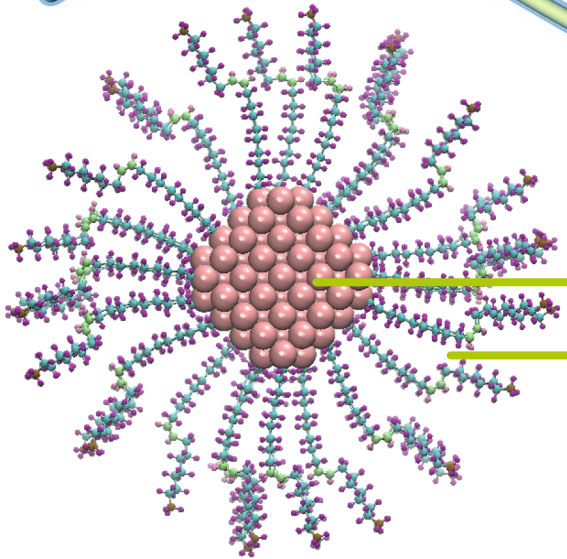


Simulation:
Dr. Hongyu Gao, Prof. Martin Müser,
Saarland University

H. Gao, TK, … M. Müser, *Nano Lett.*, 19, 10, 6993-6999, **2019**

Introduction: apolar nanoscale colloids

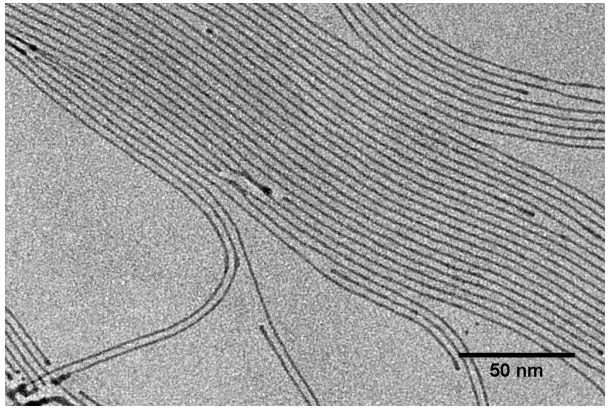




Gold

Oleylamine

n-Hexane



Simulation:
Dr. Hongyu Gao, Prof. Martin Müser,
Saarland University

H. Gao, TK, … M. Müser, *Nano Lett.*, 19, 10, 6993-6999, **2019**

Structure of this talk

1. Assembling wires

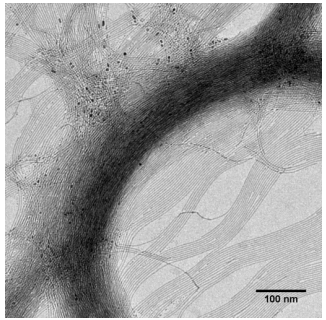
- Entropic agglomeration
- Weaving hierarchical fibres

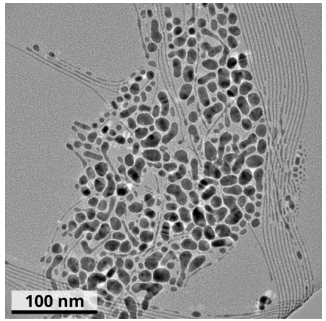
2. Stability of wires

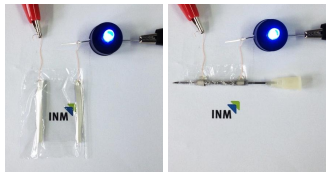
- Fragmentation via Rayleigh-Plateau
- Stabilization mechanisms

3. Transparent flexible electrodes

- Printing wires as electrodes
- Are wires or spheres better?

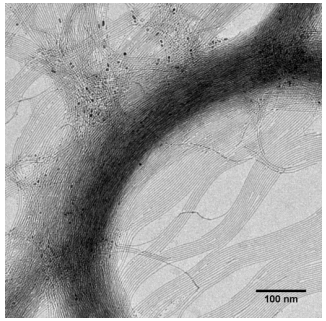


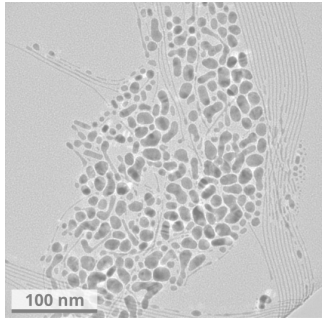


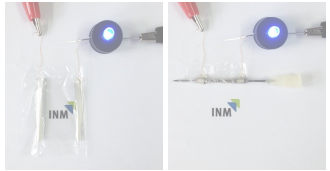


Structure of this talk

1. Assembling wires
   - Entropic agglomeration
   - Weaving hierarchical fibres
2. Stability of wires
   - Fragmentation via Rayleigh-Plateau
   - Stabilization mechanisms
3. Transparent flexible electrodes
   - Printing wires as electrodes
   - Are wires or spheres better?

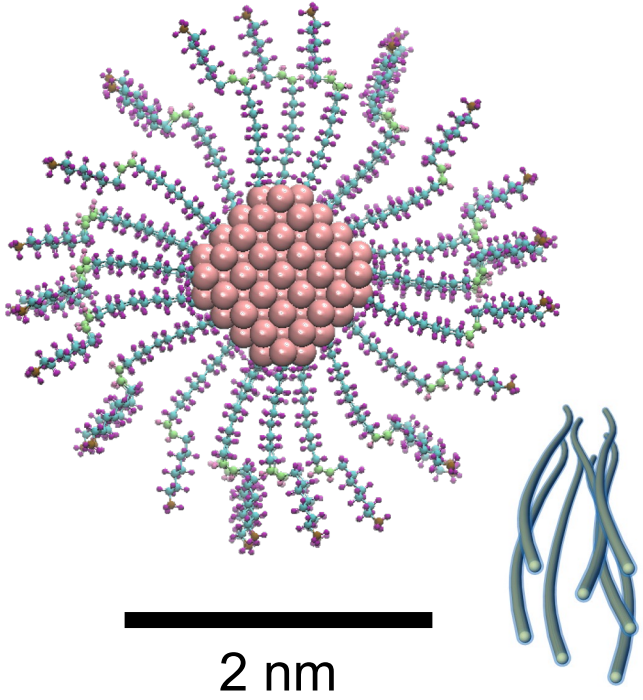


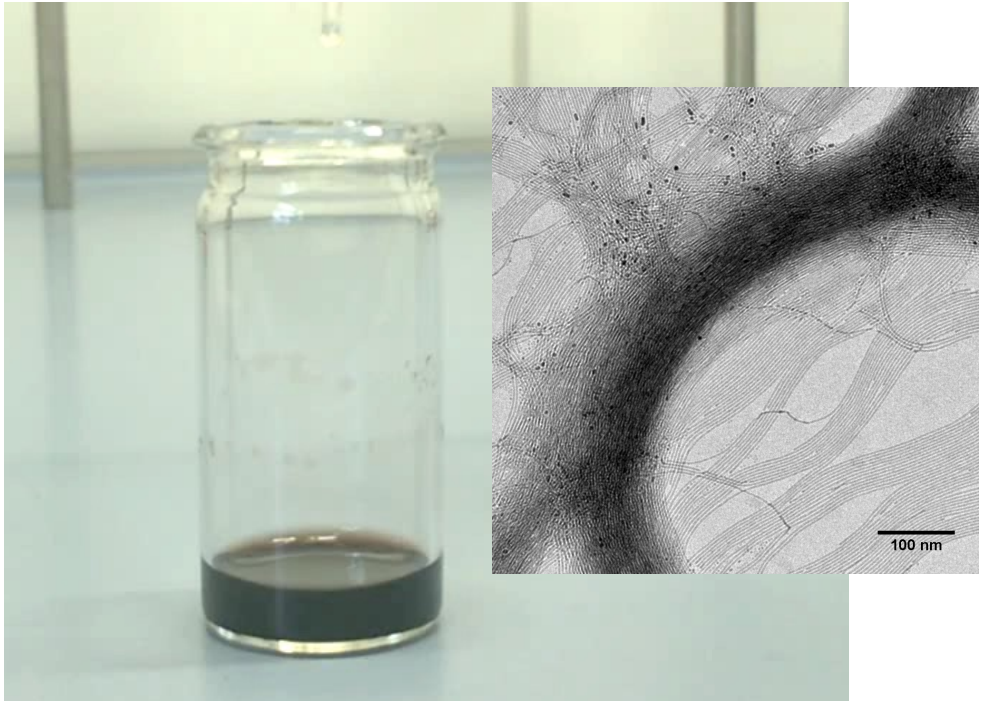




1. Assembling wires

Agglomeration in ethanol

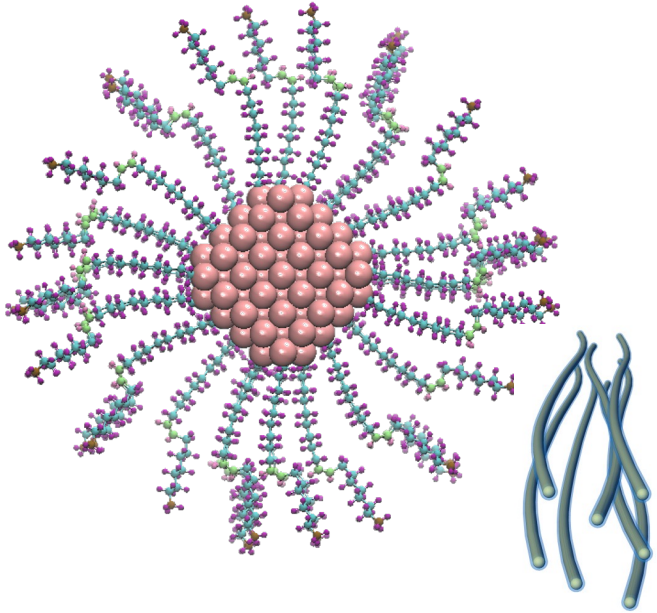


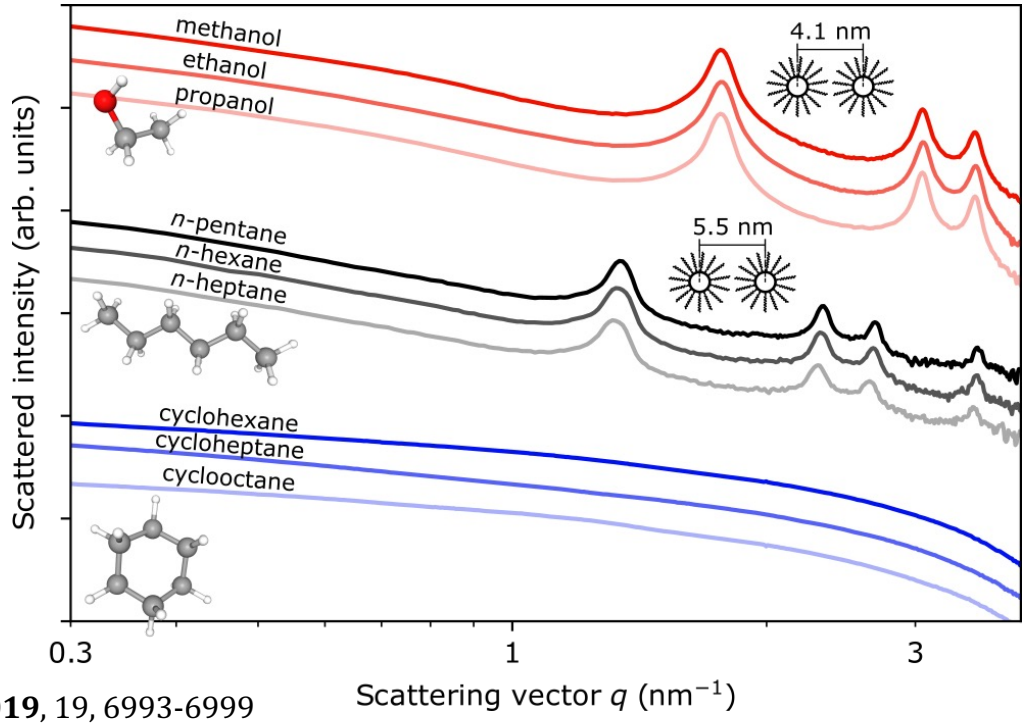


1. Assembling wires

Spacing in different solvents

Simon Bettscheider

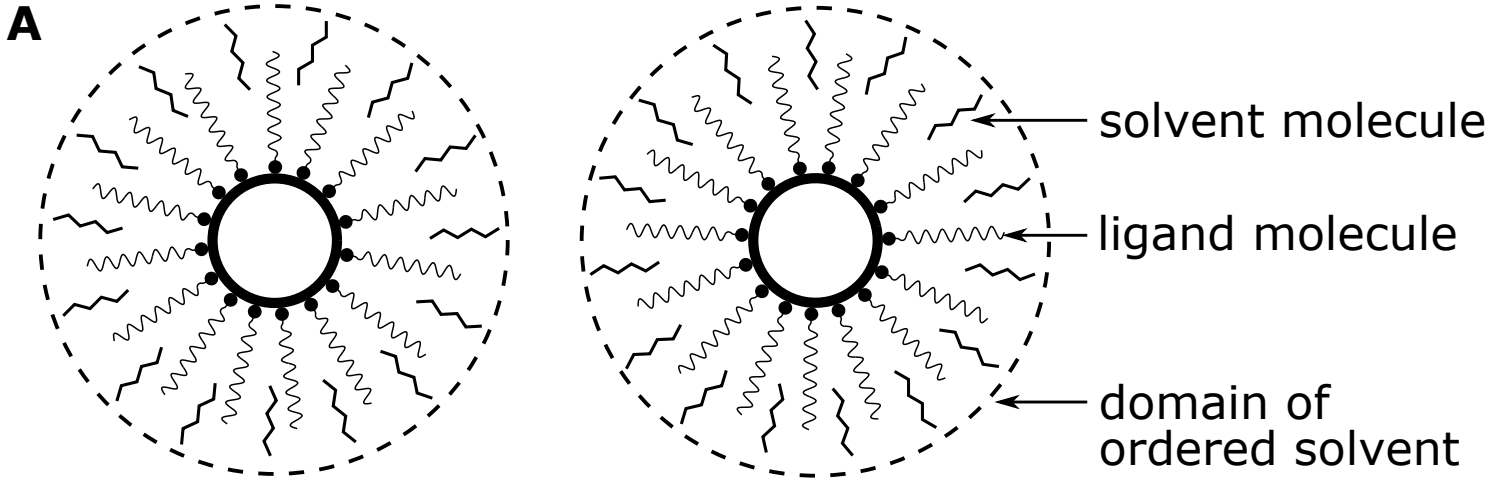




H. Gao, S. Bettscheider, TK, M.H. Müser, *Nano Letters,* **2019**, 19, 6993-6999
B. Reiser, TK, *et al., Physical Chemistry Chemical Physics* **2016**, 18, 27165-27169

1. Assembling wires

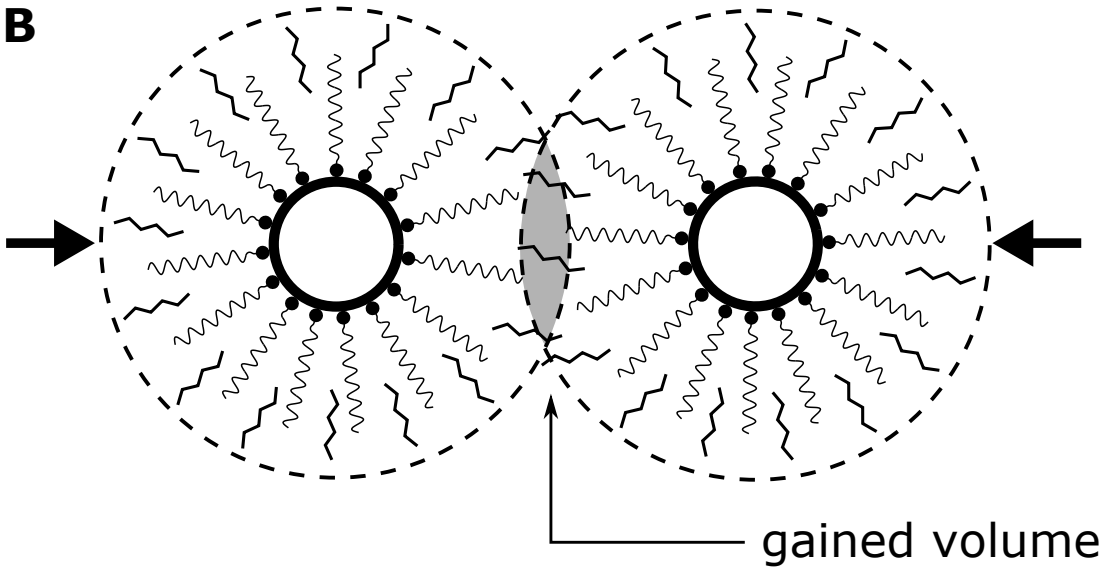
Entropic bundling



H. Gao, S. Bettscheider, T. Kraus, M.H. Müser, *Nano Letters,* **2019**, 19, 6993-6999

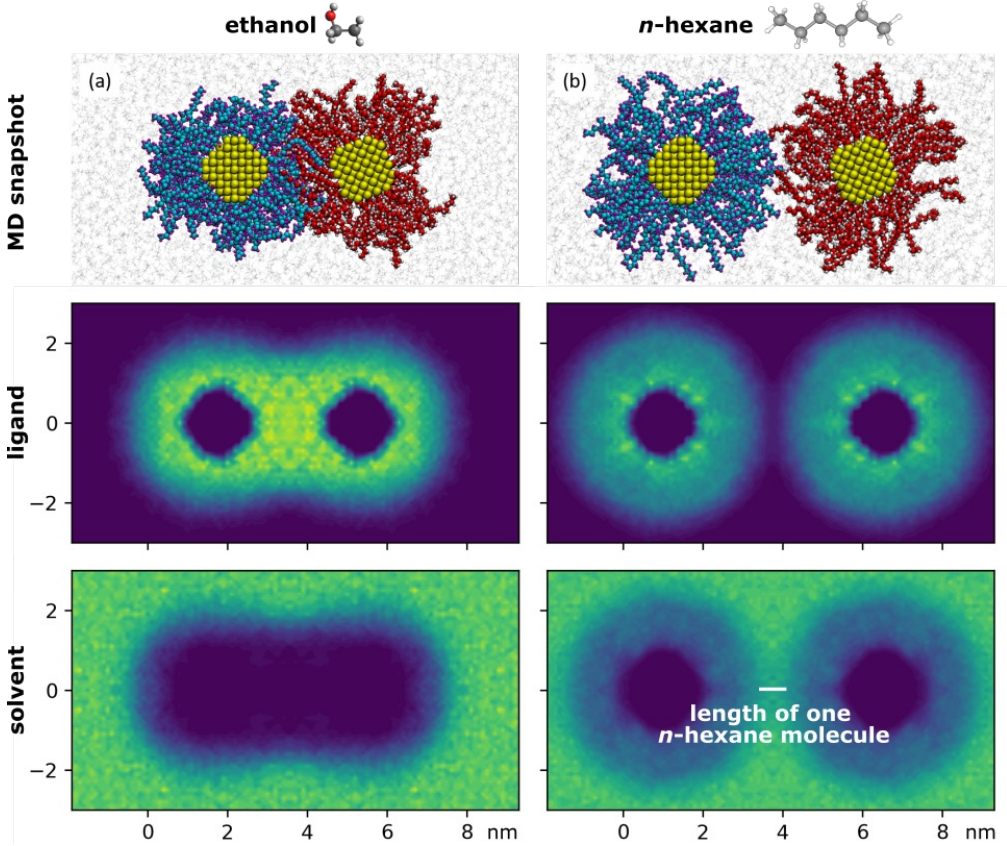
1. Assembling wires

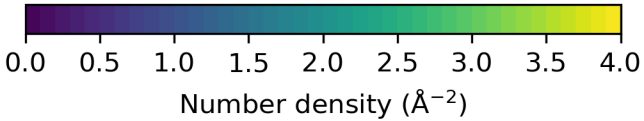
Entropic bundling



H. Gao, S. Bettscheider, T. Kraus, M.H. Müser, *Nano Letters,* **2019**, 19, 6993-6999

1. Assembling wires





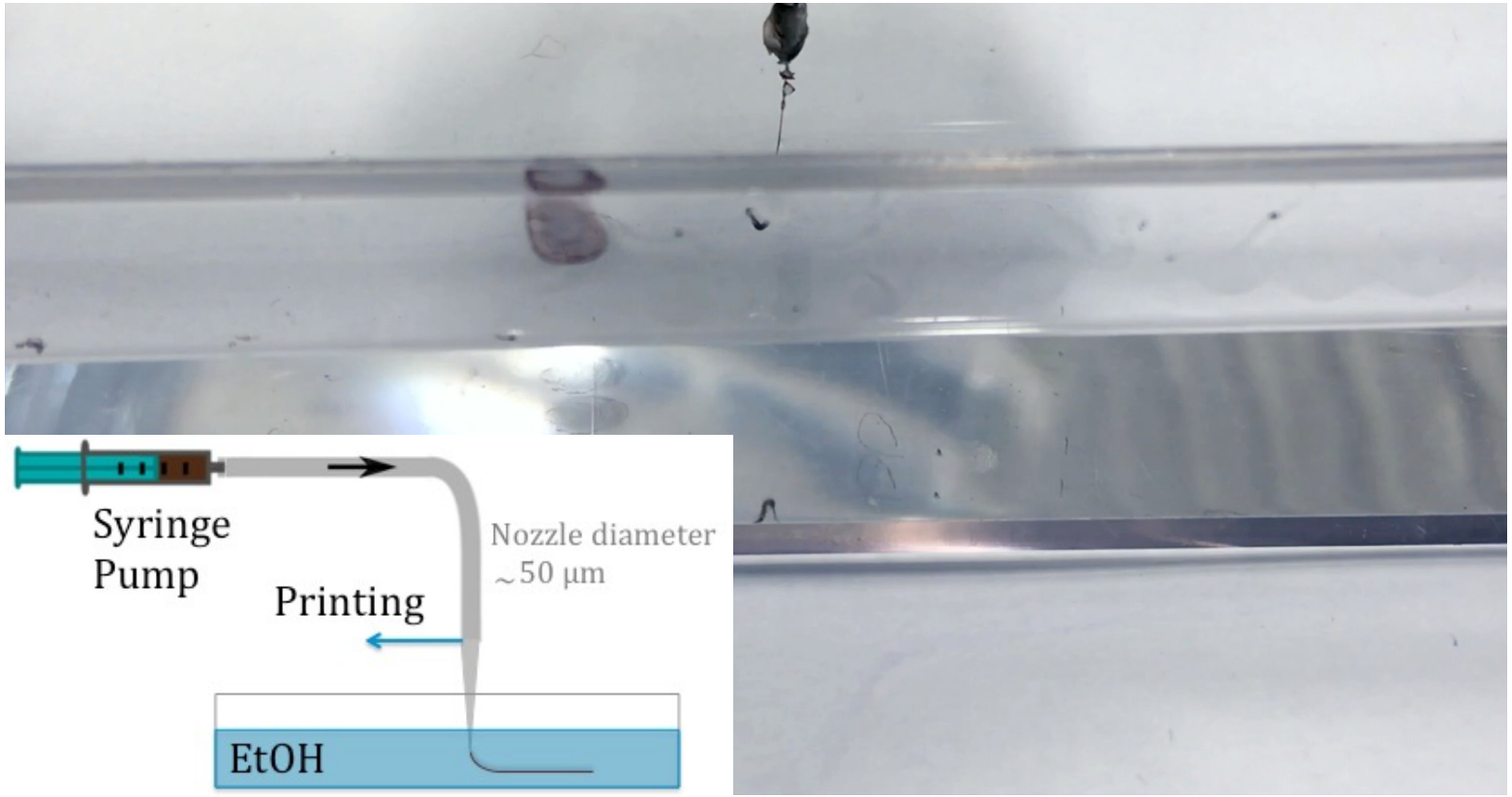
- „Bad“ solvents: exclusion from overlapping shells
- „Good“ solvents: interdigitation
- Alkanes: local ordering and „entropic bridging“

Simulations:

Dr. Hongyu Gao, Prof. Martin Müser, Saarland University

H. Gao, TK, *et al.*, *Nano Letters*, **2019**, 19, 6993-6999

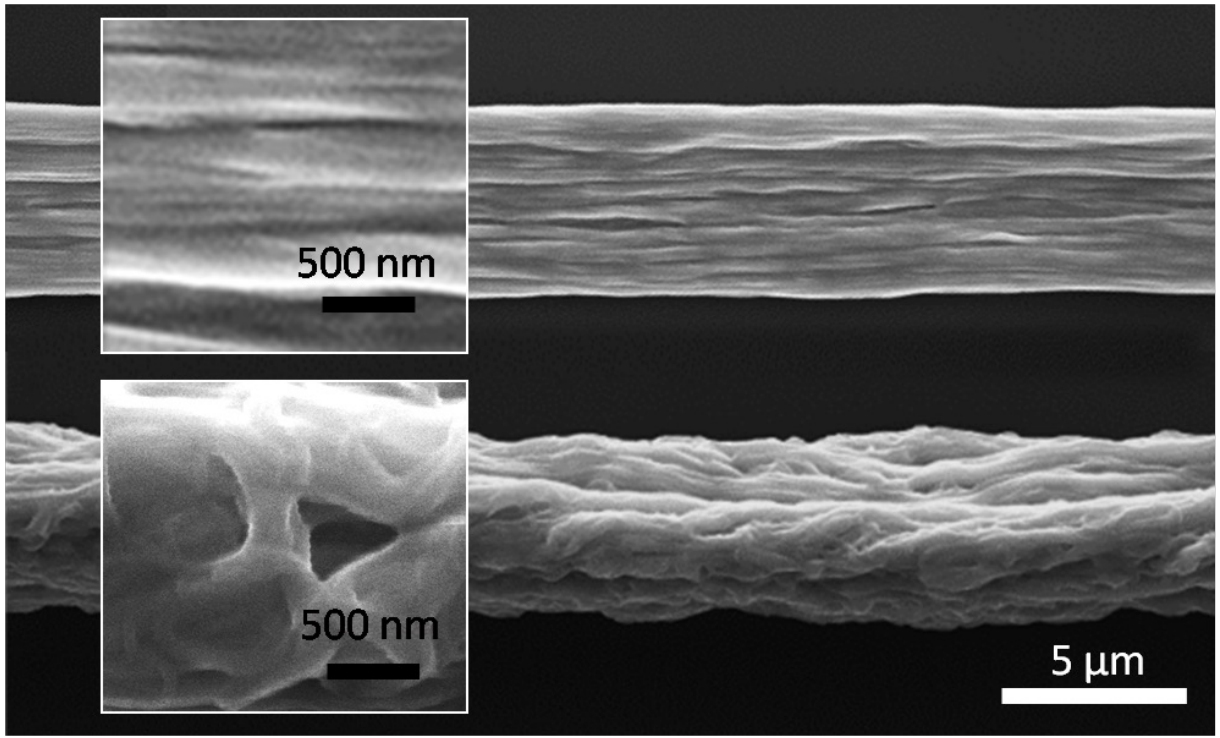
1. Assembling wires



B. Reiser *et al.*, *ACS Nano* **2017**, 11, 4934-4942

1. Assembling wires

Hierarchical bundles of wires



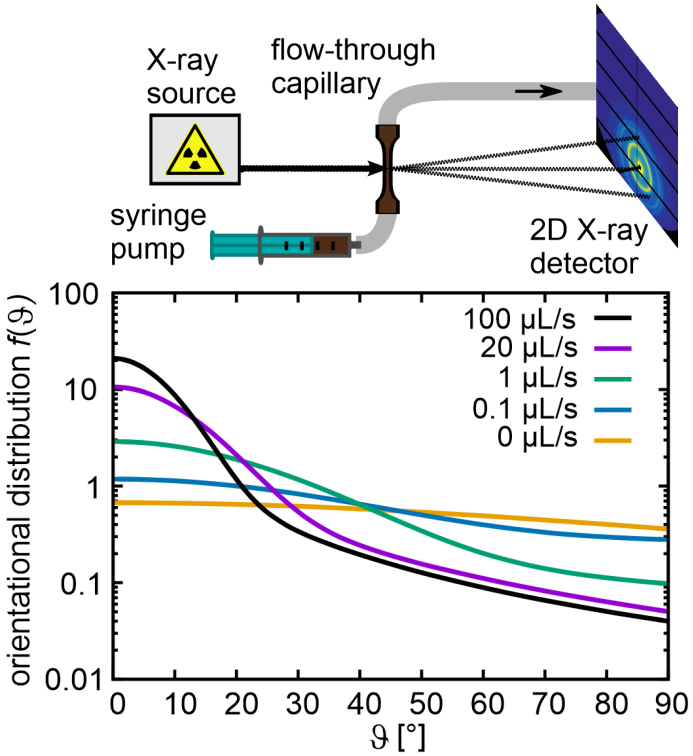
More order

Less order

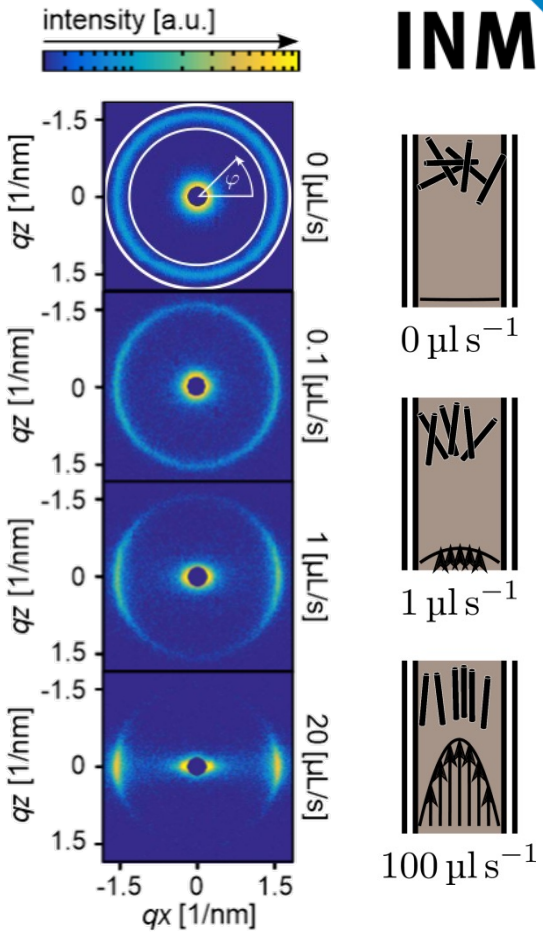
Beate Reiser

1. Assembling wires

Alignment and „spinning“ of wires

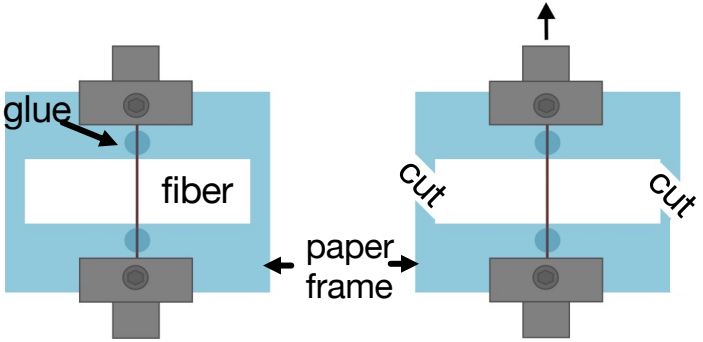


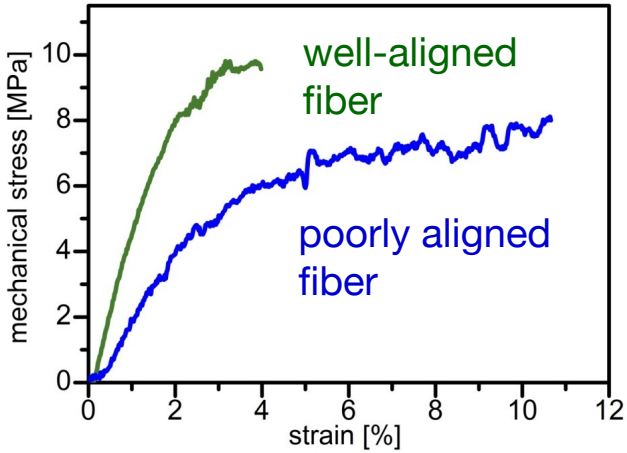
B. Reiser *et al.*, *ACS Nano* **2017**, 11, 4934-4942



1. Assembling wires

Hierarchical bundles of wires

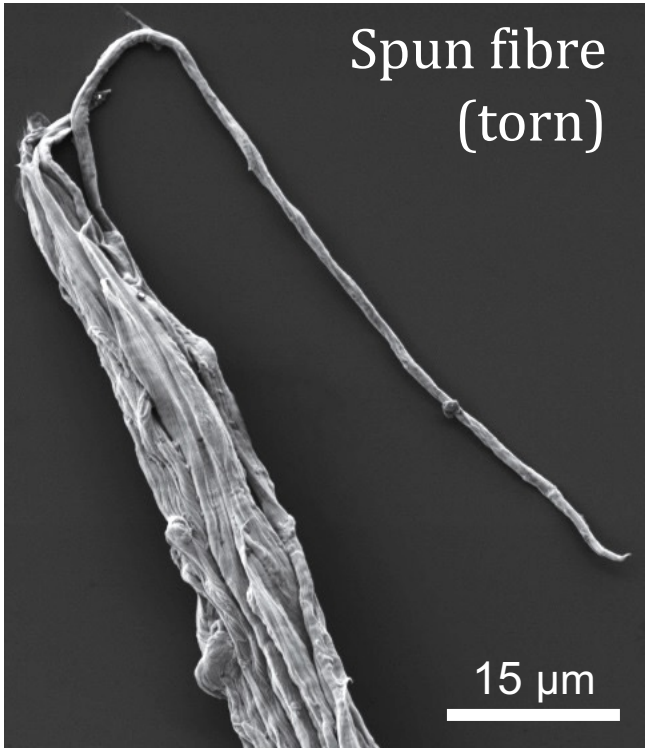




Tensile properties:

breaking stress:	10 MPa	8 MPa
strain at break :	4 %	11 %

1. Assembling wires



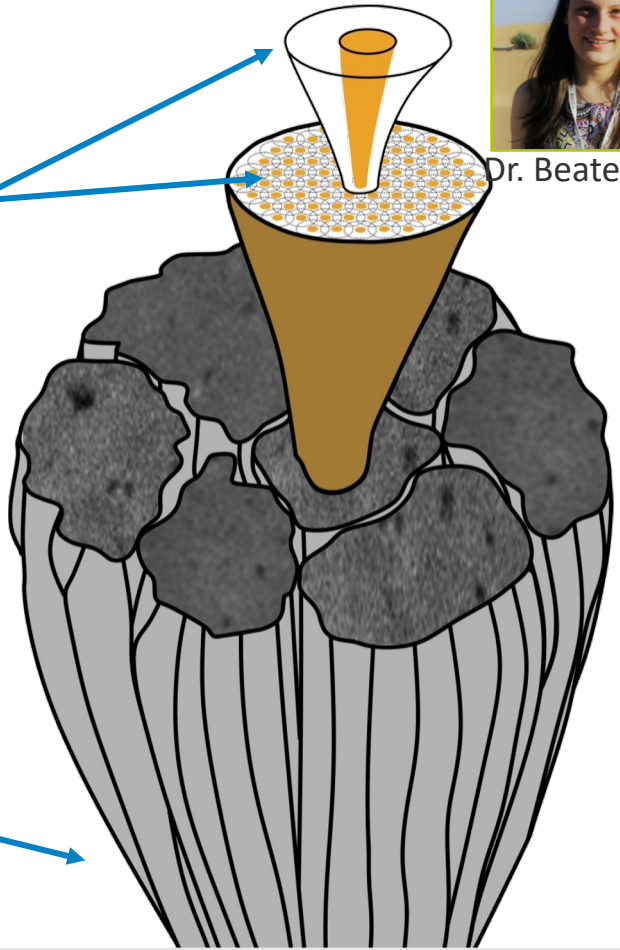
B. Reiser, …, TK, *ACS Nano* **2017**, 11, 4934-4942

Dr. Beate Reiser

single AuNWs
1.6 nm

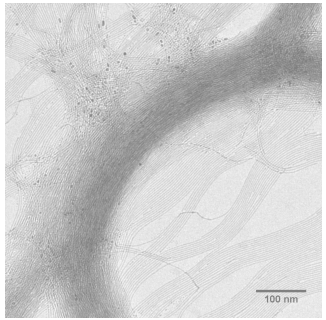
AuNW
bundles and
super-bundles
100-1000 nm

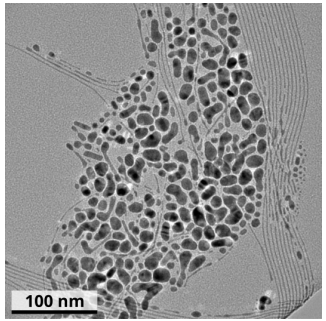
fiber
2-20 µm

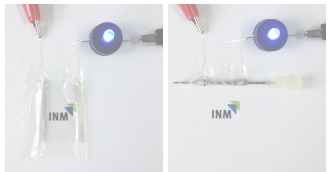


Structure of this talk

1. Assembling wires
   - Entropic agglomeration
   - Weaving hierarchical fibres
2. Stability of wires
   - Fragmentation via Rayleigh-Plateau
   - Stabilization mechanisms
3. Transparent flexible electrodes
   - Printing wires as electrodes
   - Are wires or spheres better?

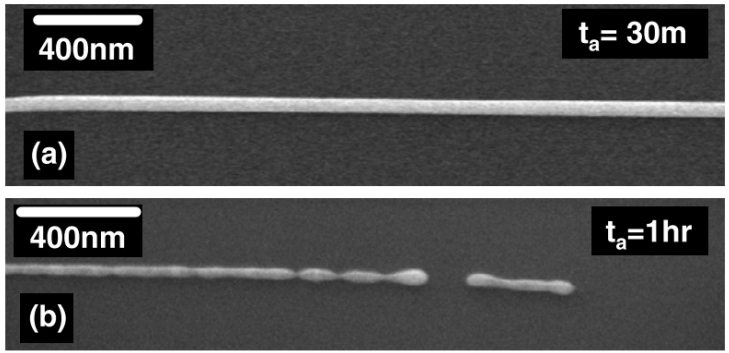




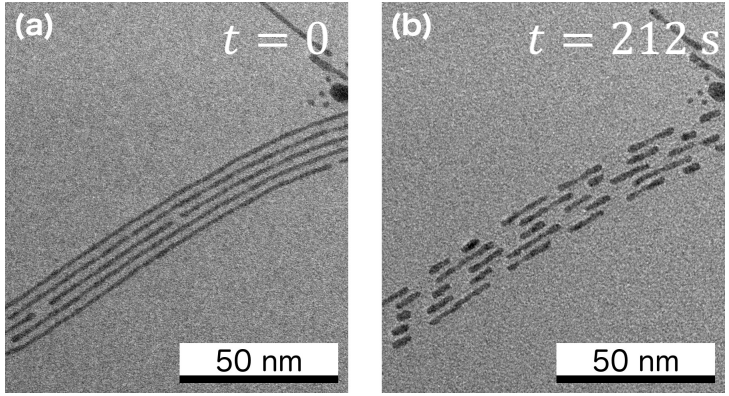


2. Stability of wires

Fragmentation via Rayleigh-Plateau Instability

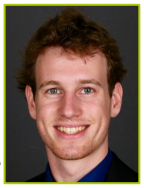


Karim et al., 2016, Nanotechnology



Bettscheider et al., 2018, J. Mech. Phys. Sol.

Simon Bettscheider



Random perturbation of wire

$$R(z,t) = R_0 + \Delta R(t) + a(t)\cos(\omega z)$$

Free energy amplifies/suppresses them

$$\Delta G = \gamma\, \Delta A$$

$\Delta G < 0$	$\Delta G \geq 0$
perturbation lowers energy	perturbation increases energy
wire will break	wire will remain cylindrical

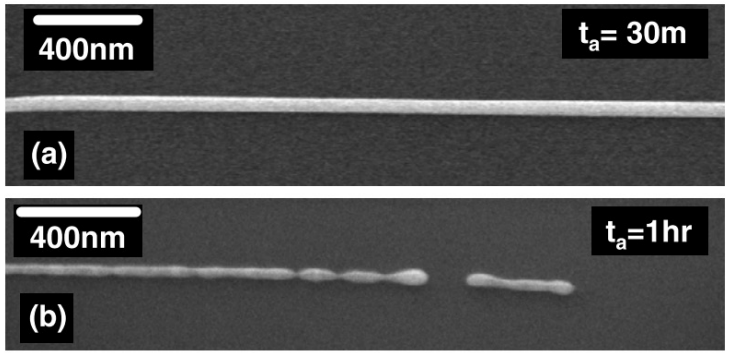
Thin wires break faster

$$t \propto R^4/\gamma$$

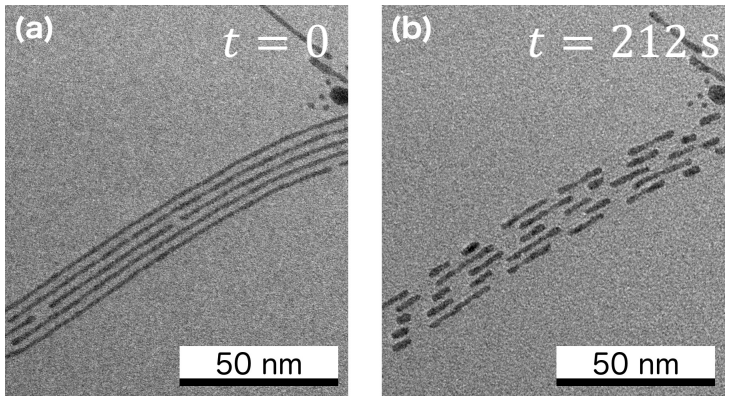
YouTube/Fluid Dynamics, CK, Abhijeet Sinha, 2016

2. Stability of wires

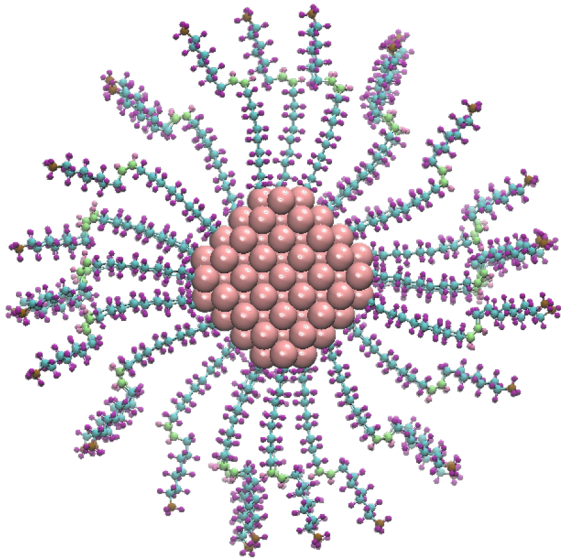
Stabilization: reduce interfacial energy



Karim et al., 2016, Nanotechnology



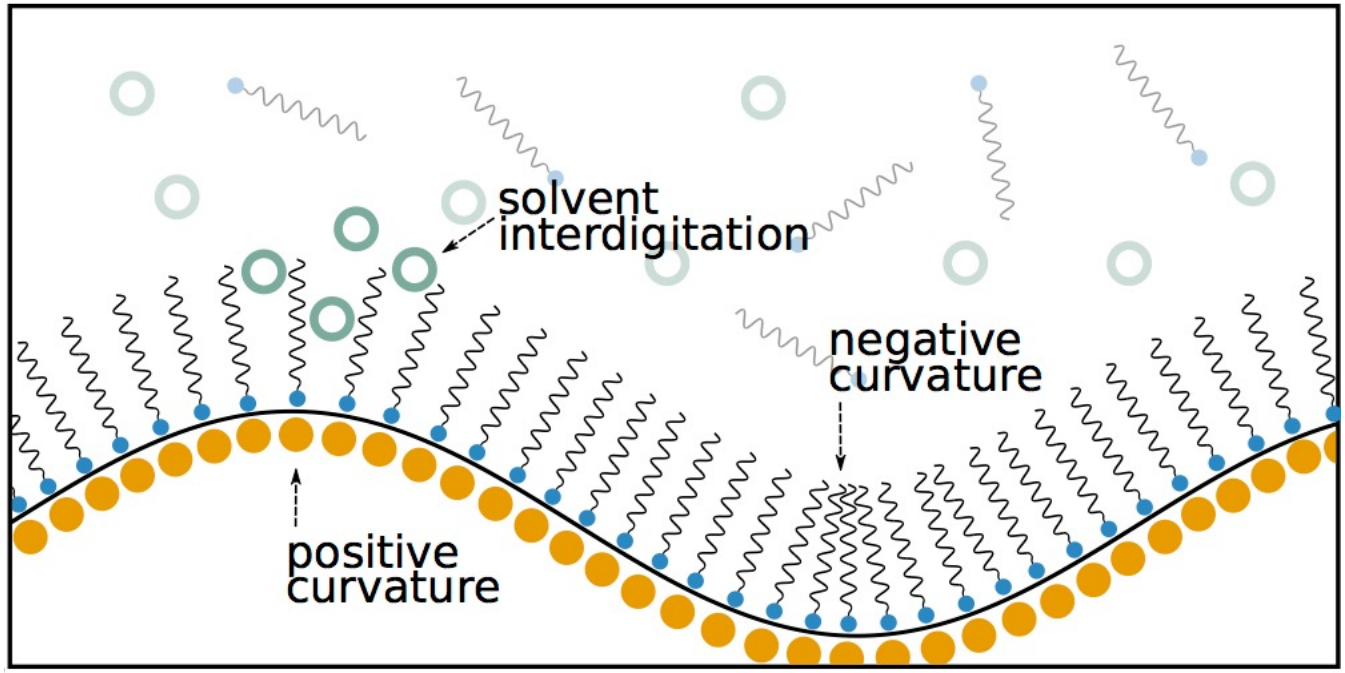
Bettscheider et al., 2018, J. Mech. Phys. Sol.



S. Bettscheider, TK, N. Fleck, *J. Mech. Phys. Sol.* **2018**, 123, 3-19

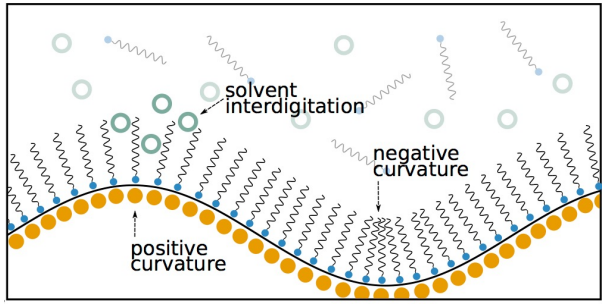
2. Stability of wires

Stabilization: reduce interfacial energy, suppress curvature



2. Stability of wires

Stabilization: reduce interfacial energy, suppress curvature



α expresses how the wires' curvature changes the effective curvature:

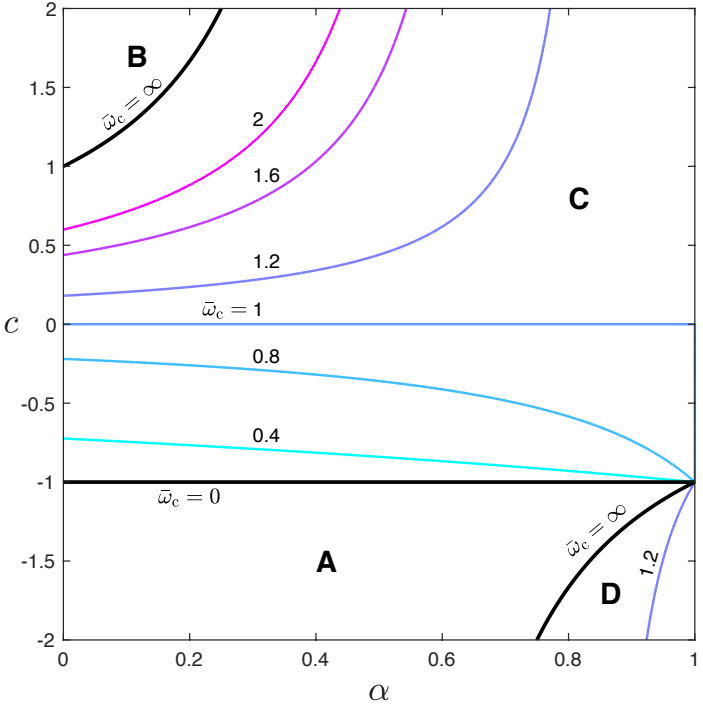
α = 1 : effective = mean curvature

α = 0 : effective = deviatoric curvature

c quantifies how the effective curvature changes interfacial energy:

c = 1 : exponential change

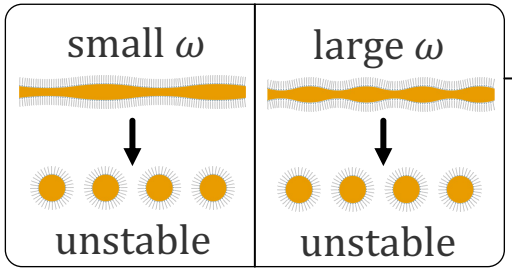
c = 0 : no change

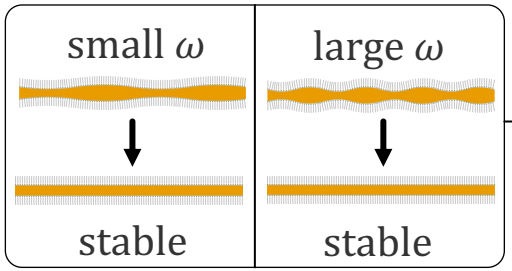


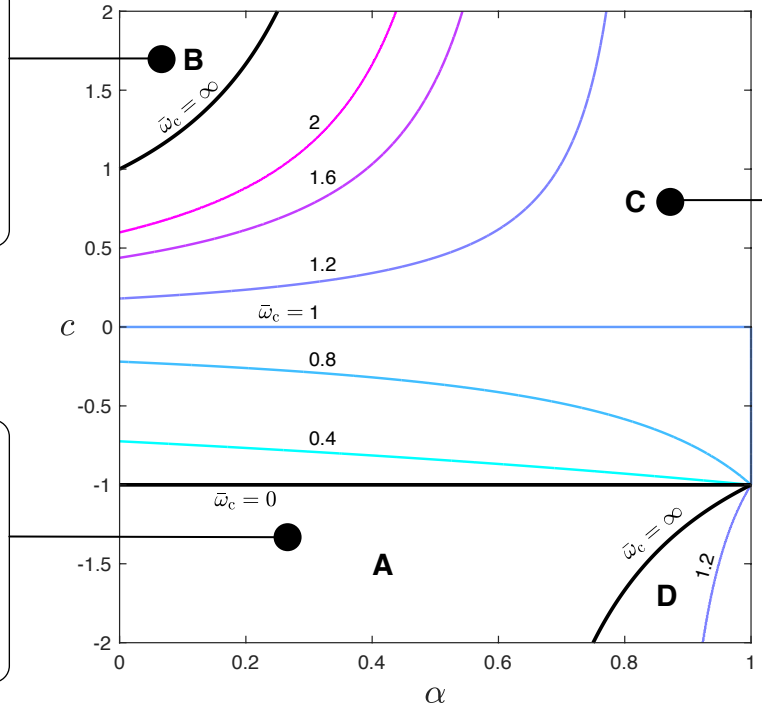
S. Bettscheider, TK, N. Fleck, *J. Mech. Phys. Sol.* **2018**, 123, 3-19

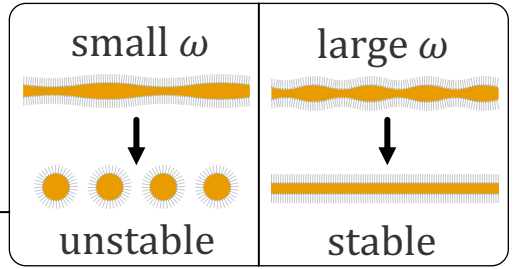
2. Stability of wires

Stabilization: reduce interfacial energy, suppress curvature









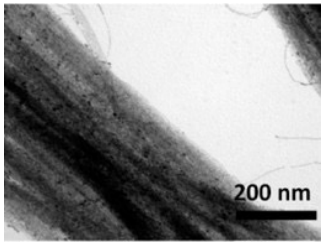
α expresses how the wires' curvature changes the effective curvature:
α = 1 : effective = mean curvature
α = 0 : effective = deviatoric curvature

c quantifies how the effective curvature changes interfacial energy:
c = 1 : exponential change
c = 0 : no change

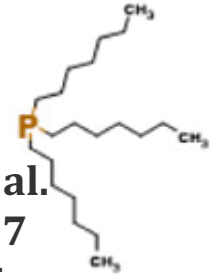
2. Stability of wires

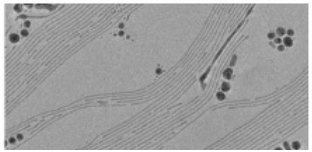
Still searching for the right molecule...

Tobias Knapp,
Yannic Curto



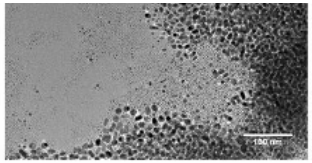
Nouh, Viao, et al.
Langmuir 2017
trioctylphosphine





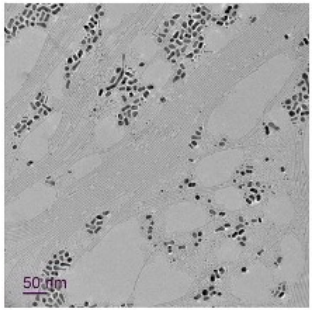
H_2N

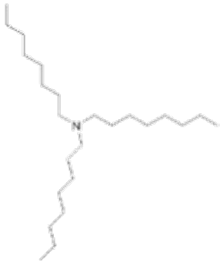
hexadecylamine



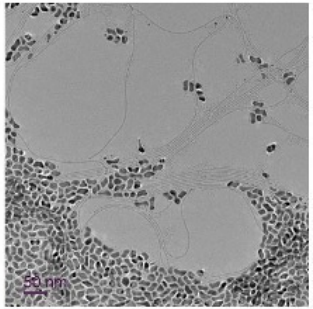
H_2N

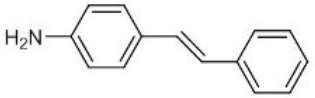
trioctylamine





dodecylamine

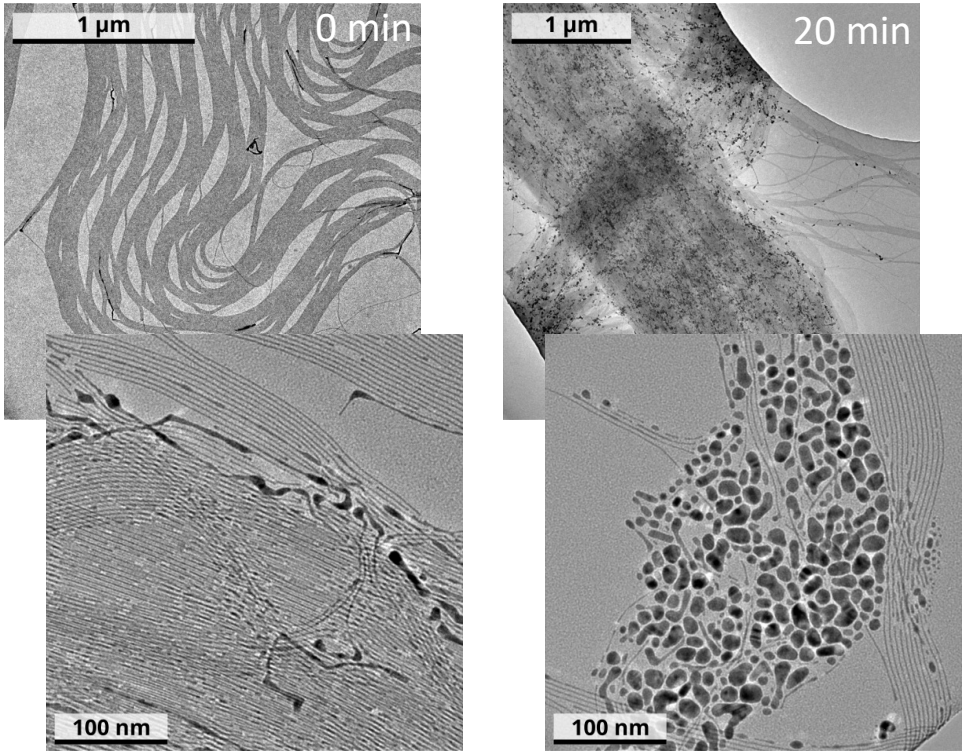


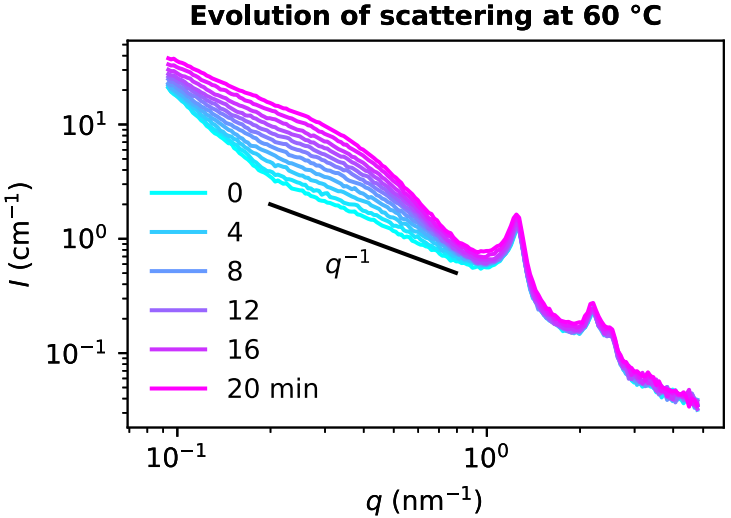


2-phenylethenylamin

2. Stability of wires

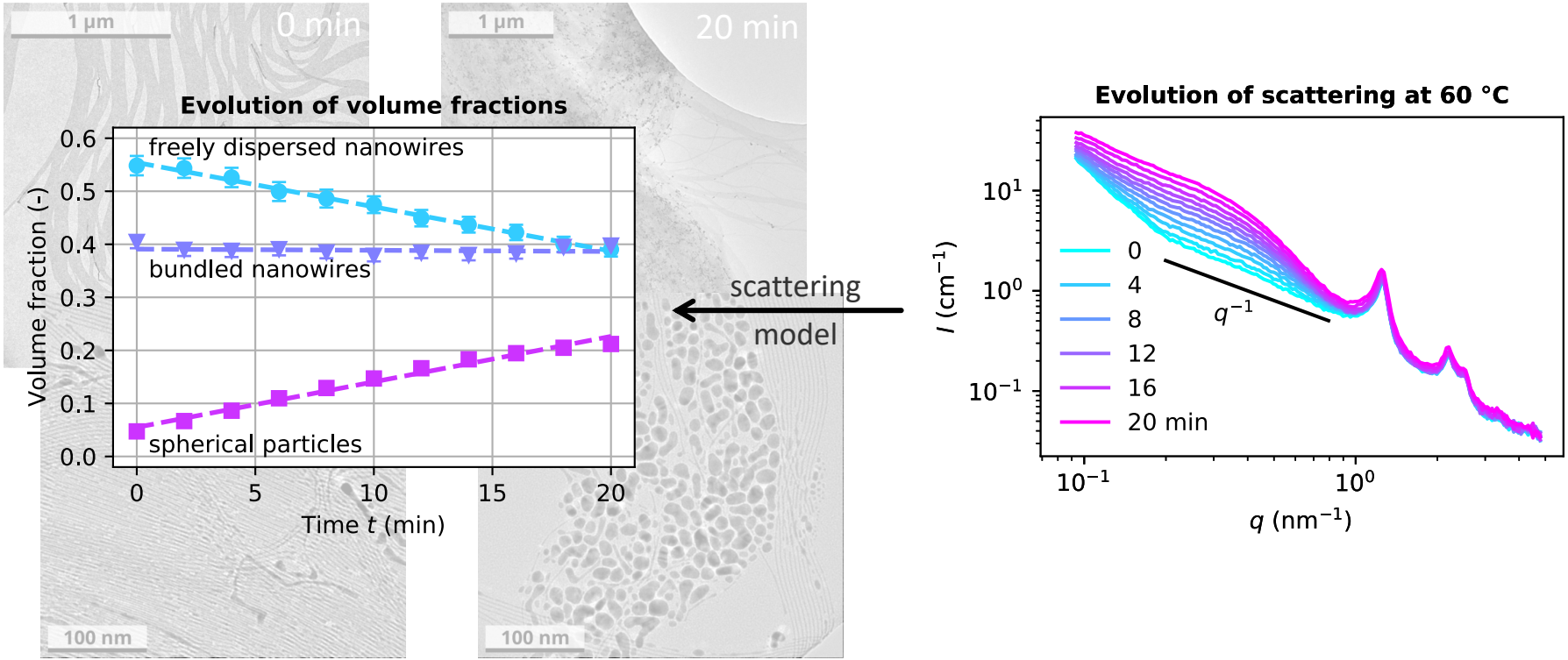
Stability of wires in bundles





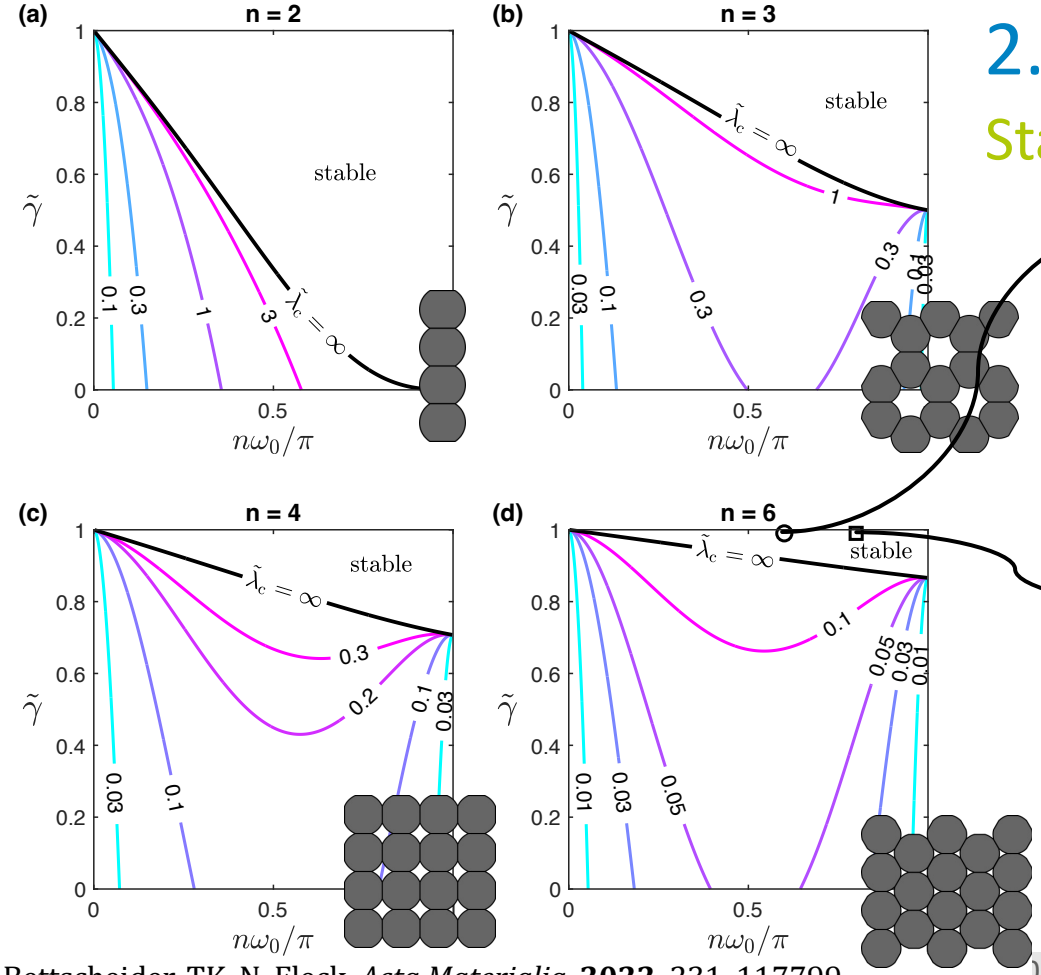
2. Stability of wires

Stability of wires in bundles



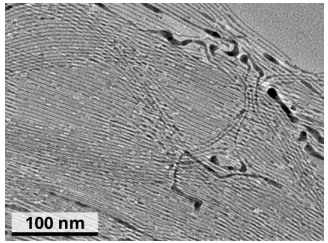
2. Stability of wires

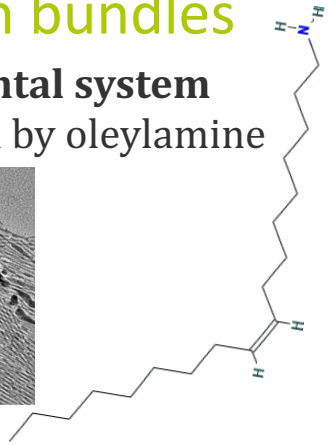
Stability of wires in bundles



Our experimental system

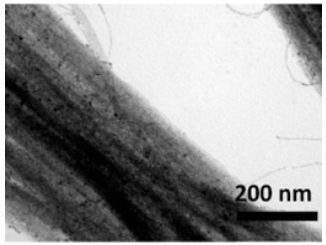
Au NWs capped by oleylamine

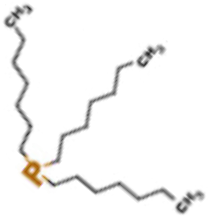




Nouh et al. Langmuir 2017

Au NWs capped by trioctylphosphine

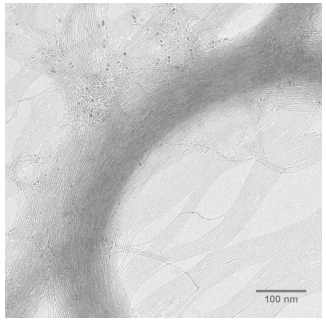


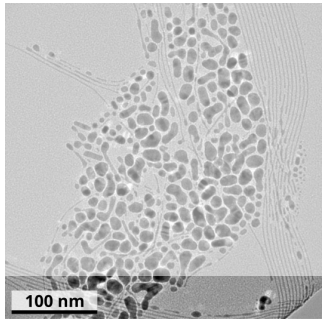


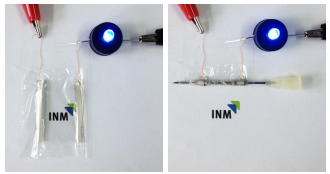
S. Bettscheider, TK, N. Fleck, *Acta Materialia.* **2022**, 231, 117799

Structure of this talk

1. Assembling wires
   - Entropic agglomeration
   - Weaving hierarchical fibres
2. Stability of wires
   - Fragmentation via Rayleigh-Plateau
   - Stabilization mechanisms
3. Transparent flexible electrodes
   - Printing wires as electrodes
   - Are wires or spheres better?

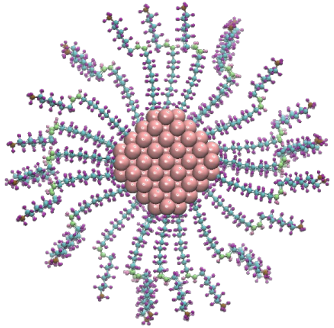


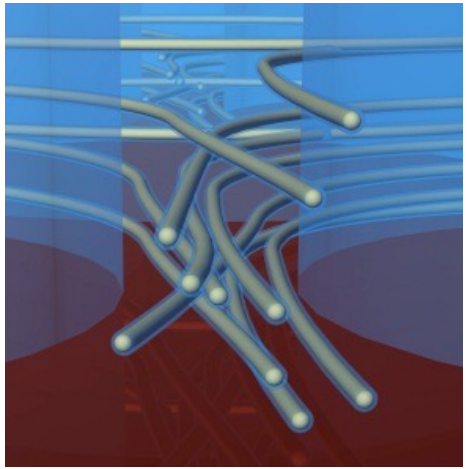




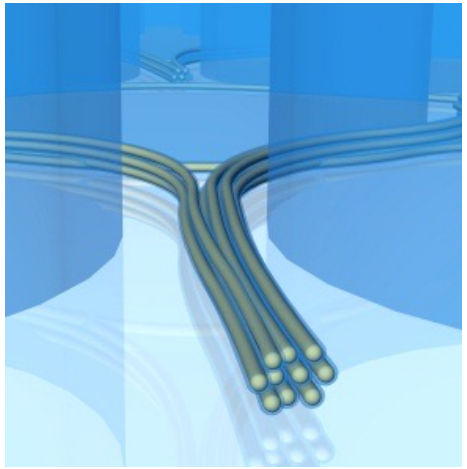
3. Transparent flexible electrodes

Printing wires as bundles

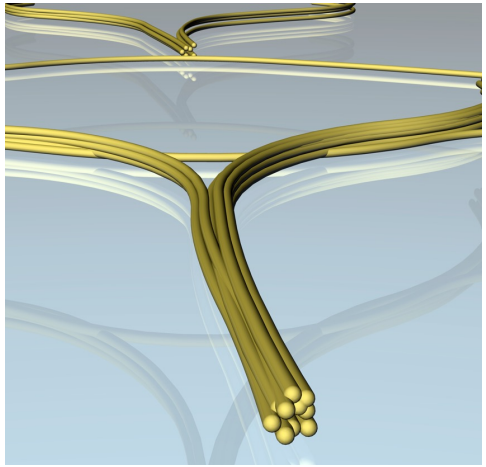




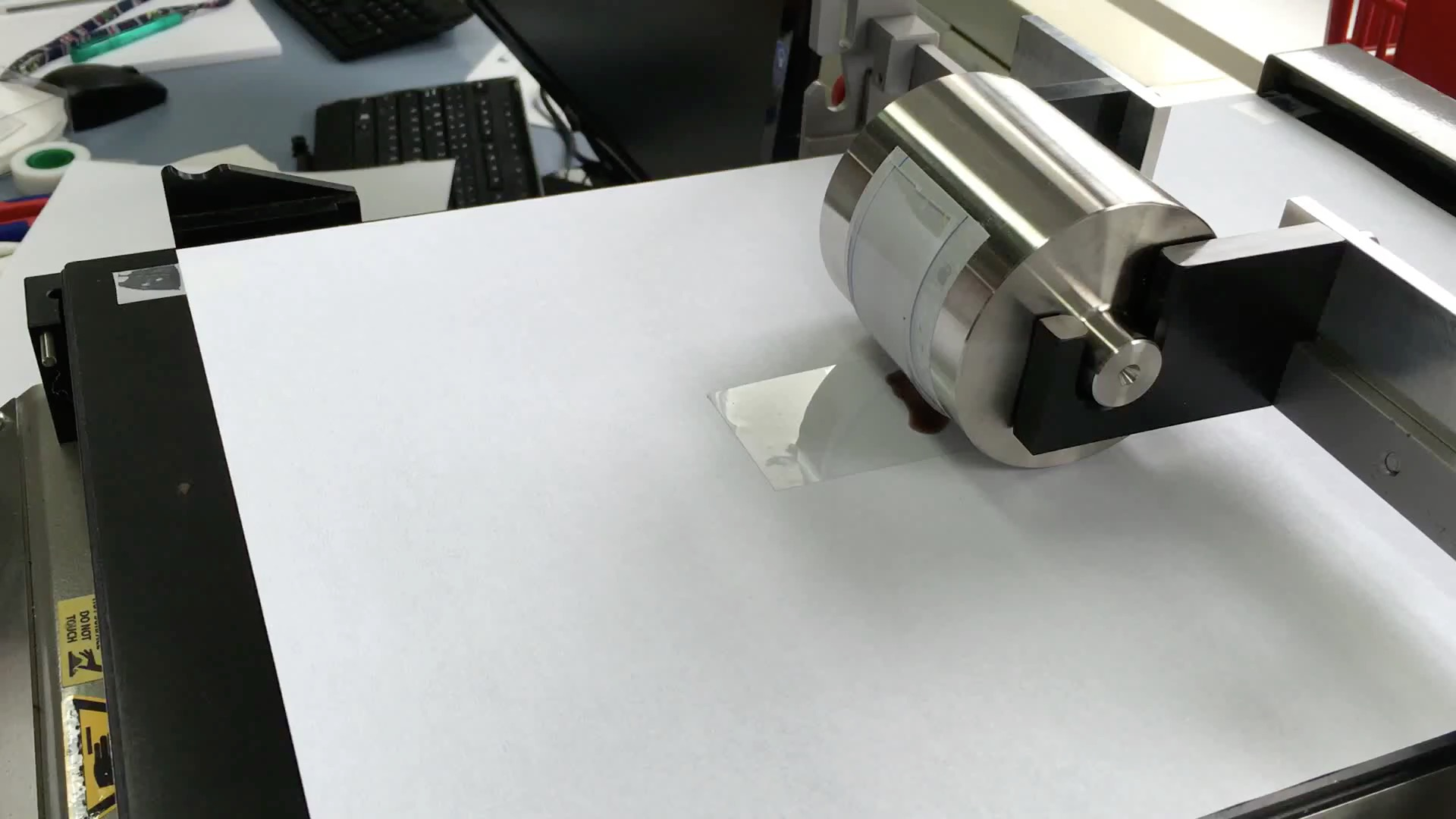
Dispersed wires confined in a stamp...



...self-assemble into hexagonal bundles...

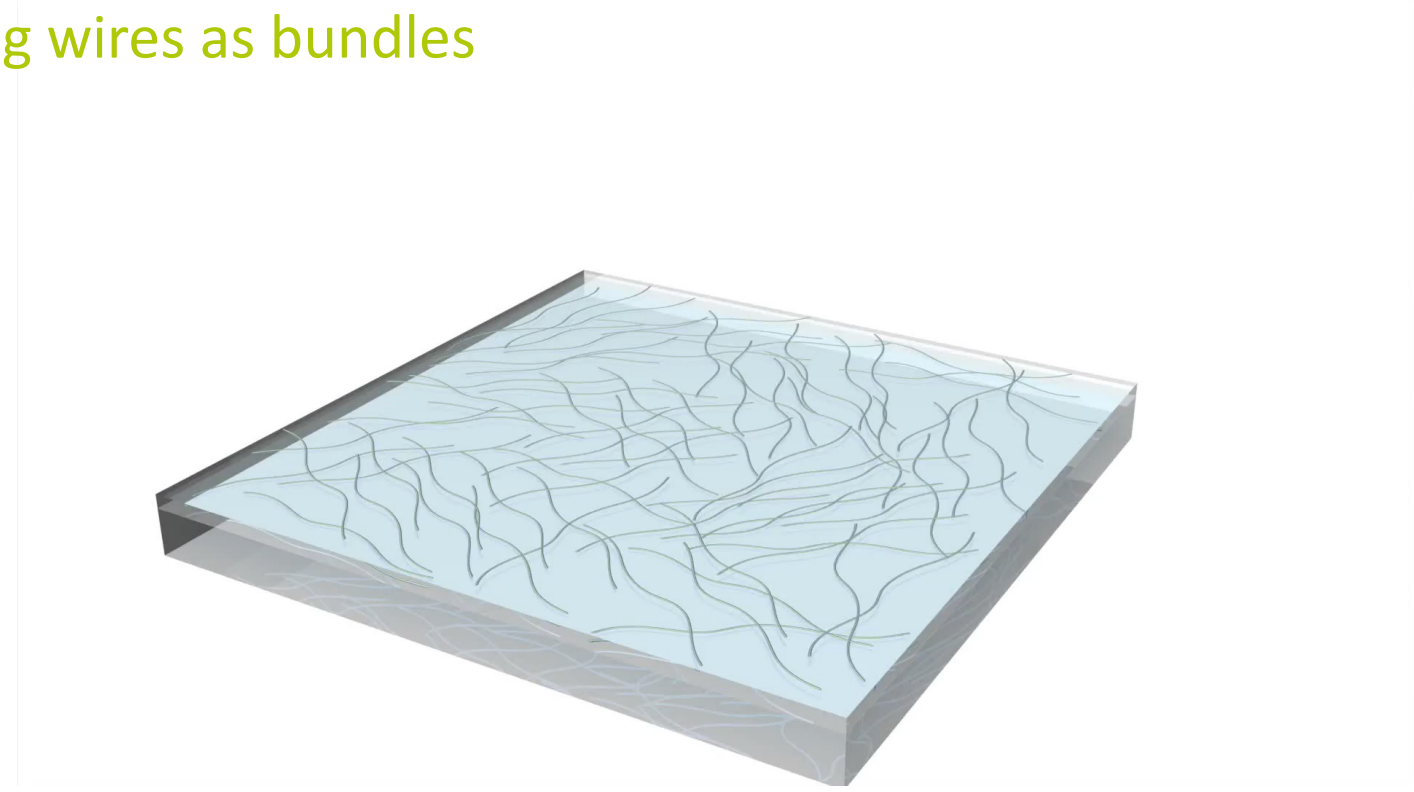


...that plasma sinters into to percolating wires.

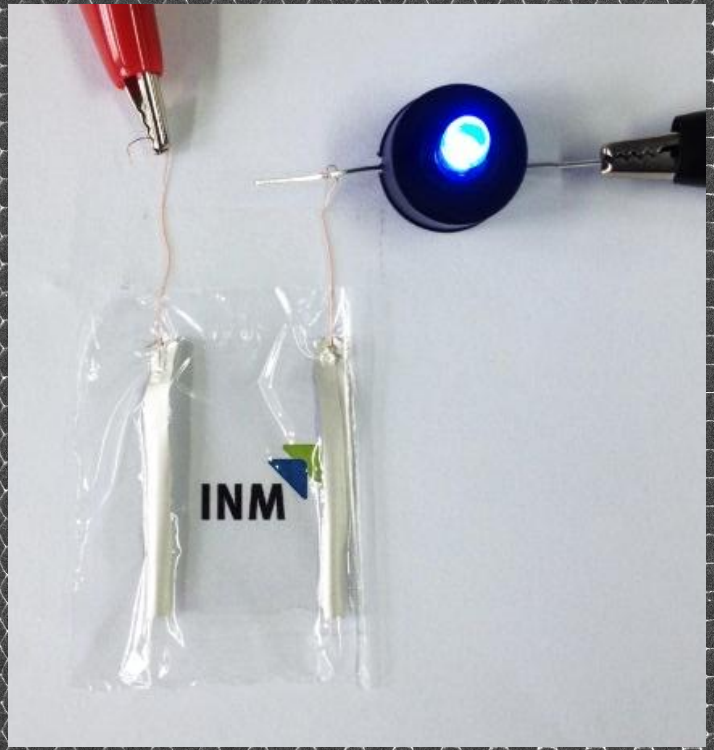

DO NOT TOUCH

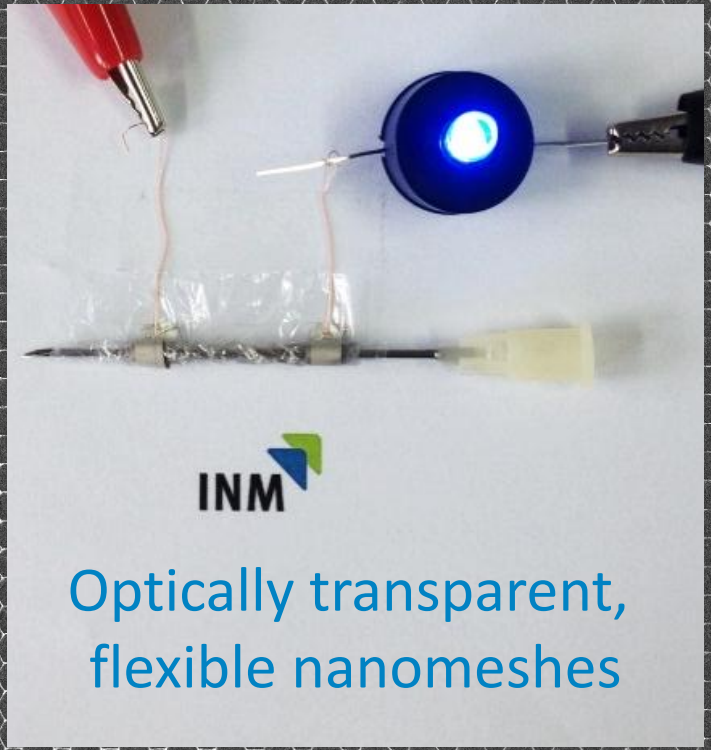
3. Transparent flexible electrodes

Printing wires as bundles



J.H.M. Maurer, TK *et al., Nano Letters* **2016**, 16 (5), 2921; INM patent filed

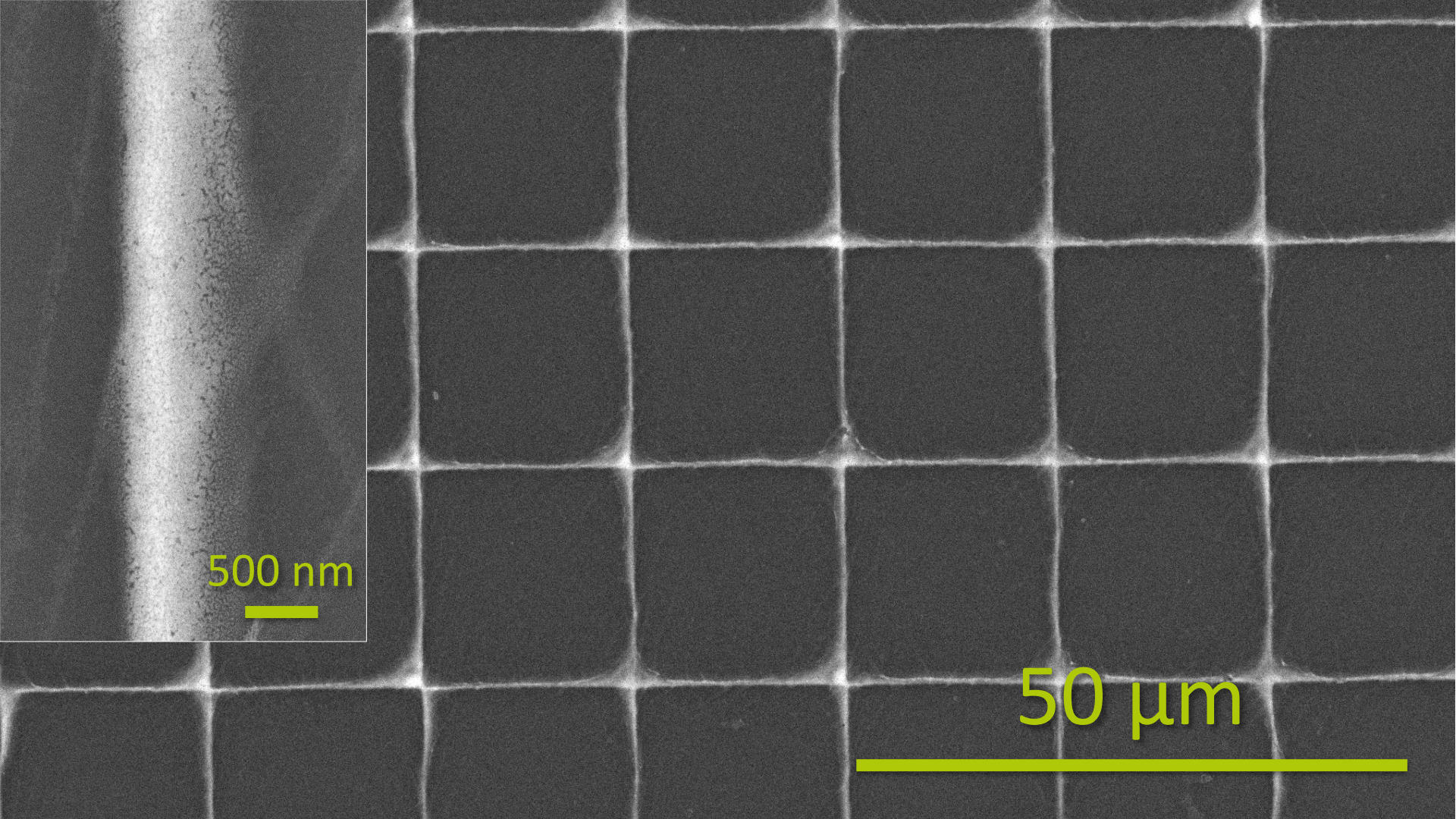




Optically transparent, flexible nanomeshes

500 µm

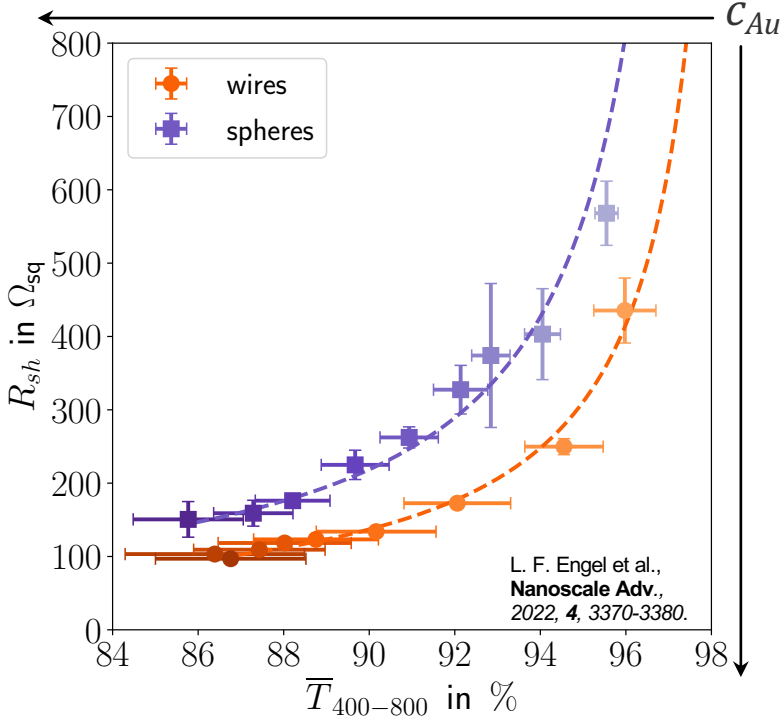
J.H.M. Maurer *et al., Nano Letters* **2016**, 16 (5), 2921

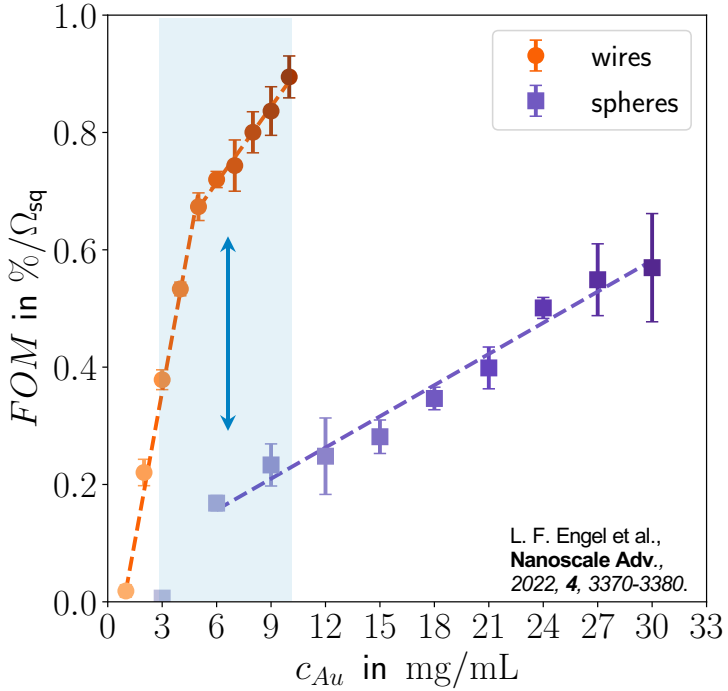

500 nm
50 µm

3. Transparent flexible electrodes

Printing wires versus spheres

Lukas F. Engel

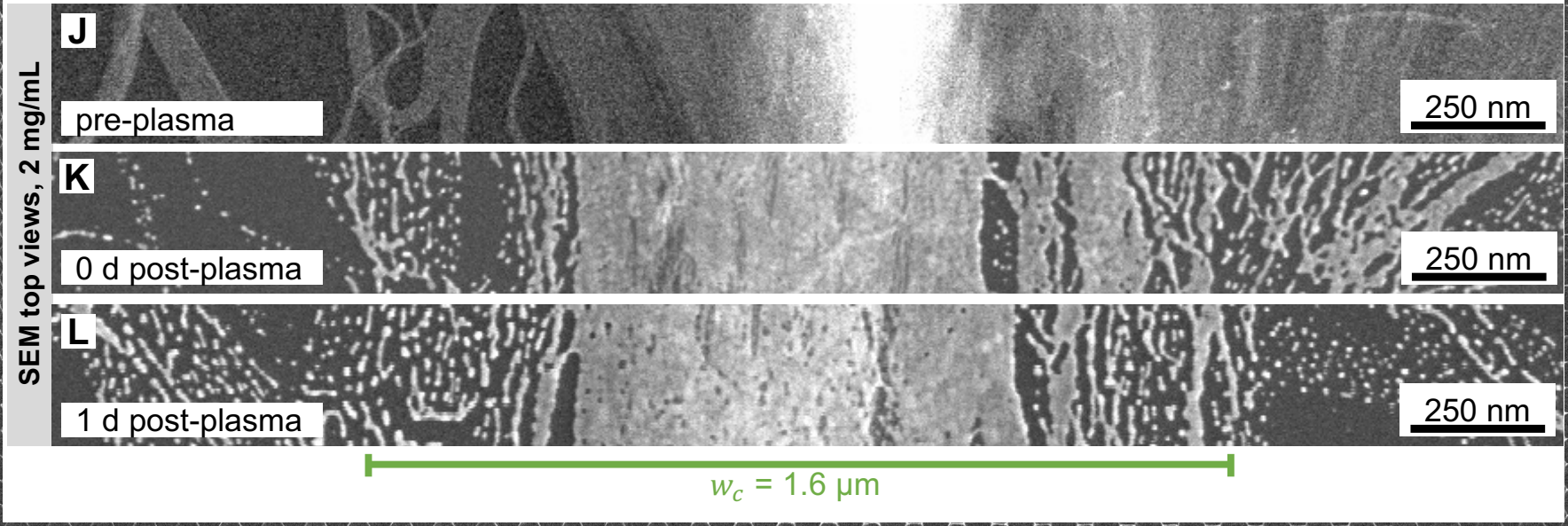




L.F. Engel, L. González-García, TK, *Nanoscale Advances* **2022**, 4, 3370-3380

3. Transparent flexible electrodes

Stability of wires in bundles



Structure of this talk

1. Assembling wires

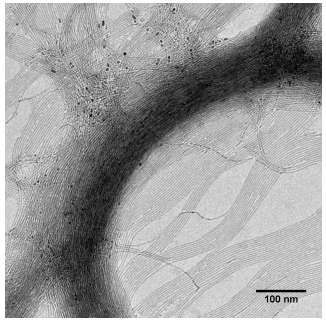
- Entropic agglomeration
- Weaving hierarchical bundles

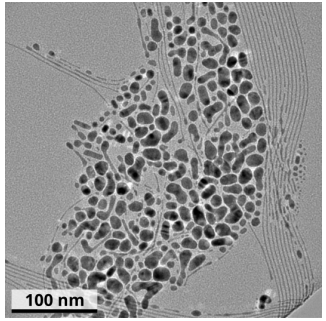
2. Stability of wires

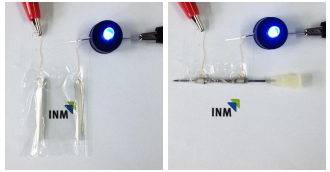
- Fragmentation via Rayleigh-Plateau
- Stabilization mechanisms

3. Transparent flexible electrodes

- Printing wires as electrodes
- Are wires or spheres better?







New Thinking. New Materials.

INM

THANK YOU VERY MUCH FOR YOUR ATTENTION

Bundesministerium für Bildung und Forschung

DFG

Bundesministerium für Wirtschaft und Energie

DAAD