1 Introduction

Table of Contents

Learning Goals

- organic chemistry is the basis of polymer science and soft matter research
- organic chemistry deals with molecular compounds of carbon
- carbon is always tetravalent
- carbon can attain different hybridization states, coordination geometries
- carbon forms single, double, triple bonds to other carbons and heteroatoms
- therefore, a vast array of binding options, molecular geometries
- carbon is always tetravalent

1.1 Organic Chemistry & Soft Matter Research

The Role of Organic Chemistry for Everyday Life

lipids

carbohydrates

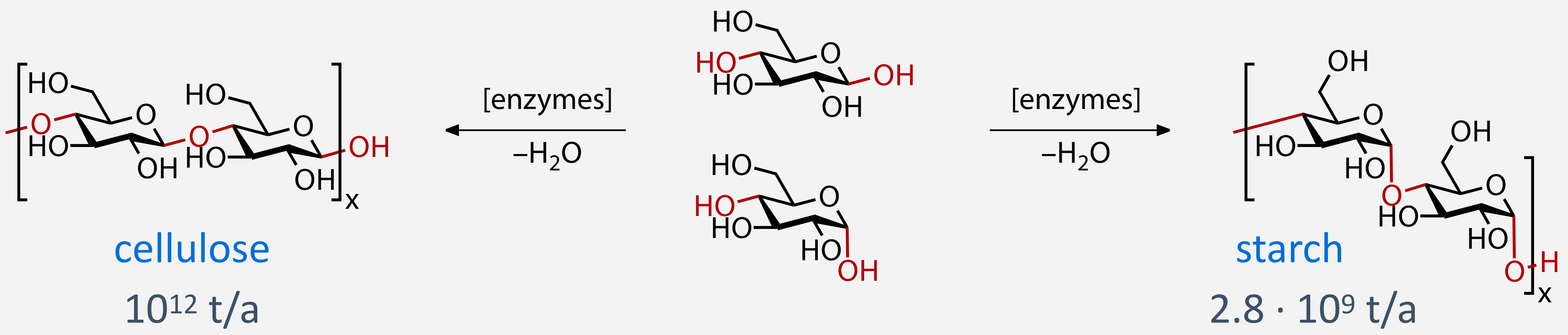
proteins

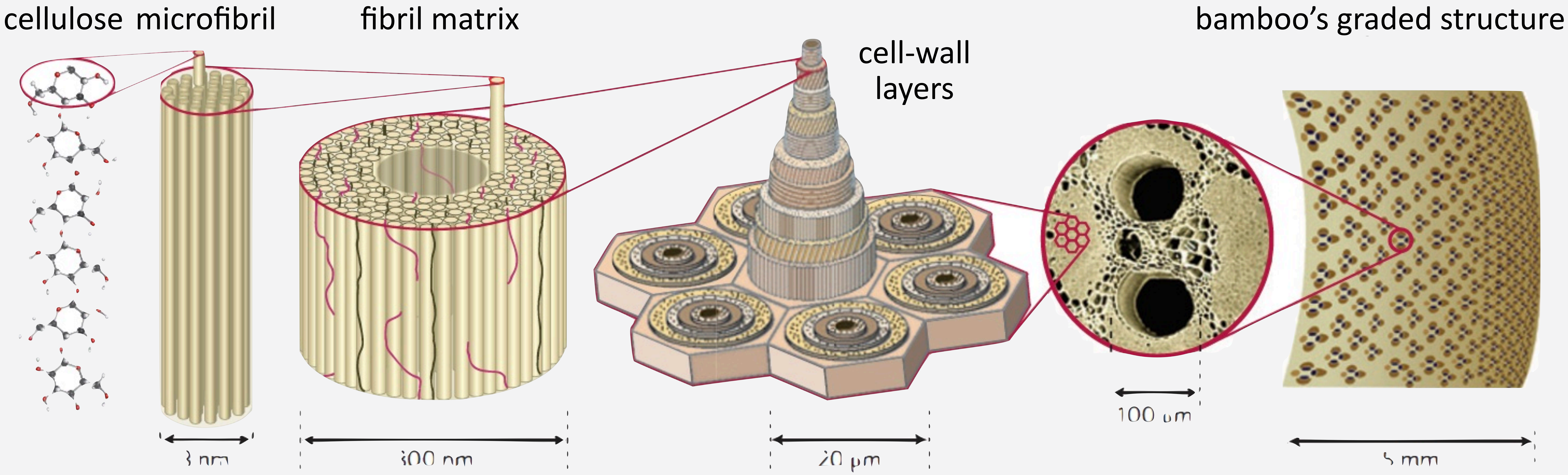
odorants

pharmaceutics

food & consumer goods

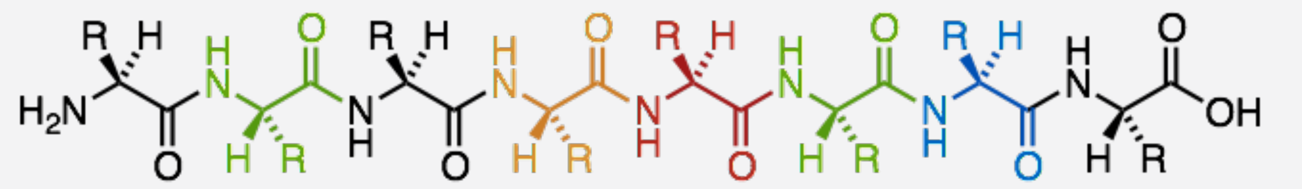
Examples of Natural Polymers: Polysaccharides

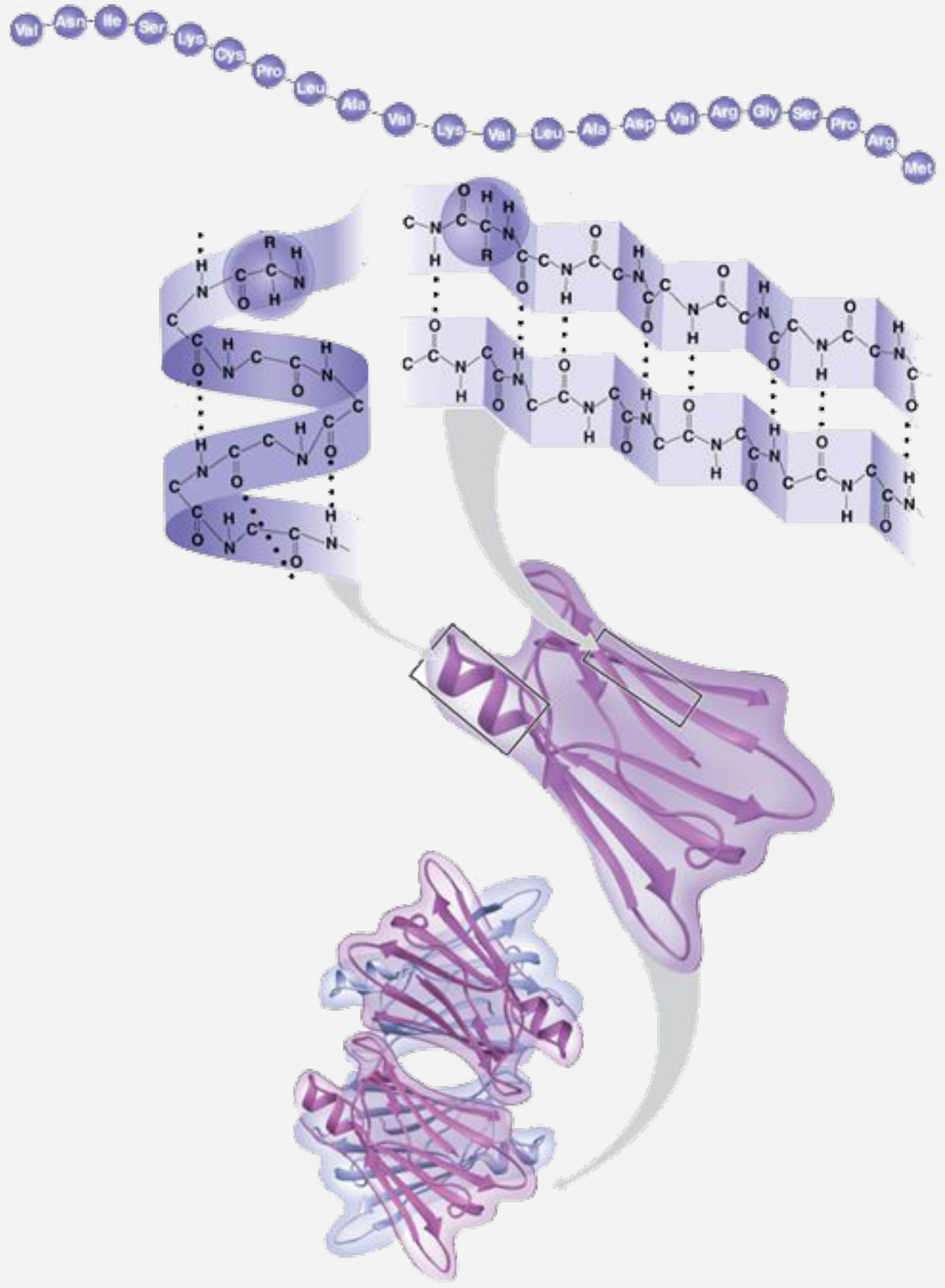




- **biomaterials: hierarchical structures on different length scales for optimized performance**

Examples of Natural Polymers: Peptides





- **Primary Structure**

  defined macromolecule from 20 amino acids

- **Secondary Structure**

  3D form of local segments (α-helices, β-sheets) as the result of defined patterns of hydrogen bonds

- **Tertiary Structure**

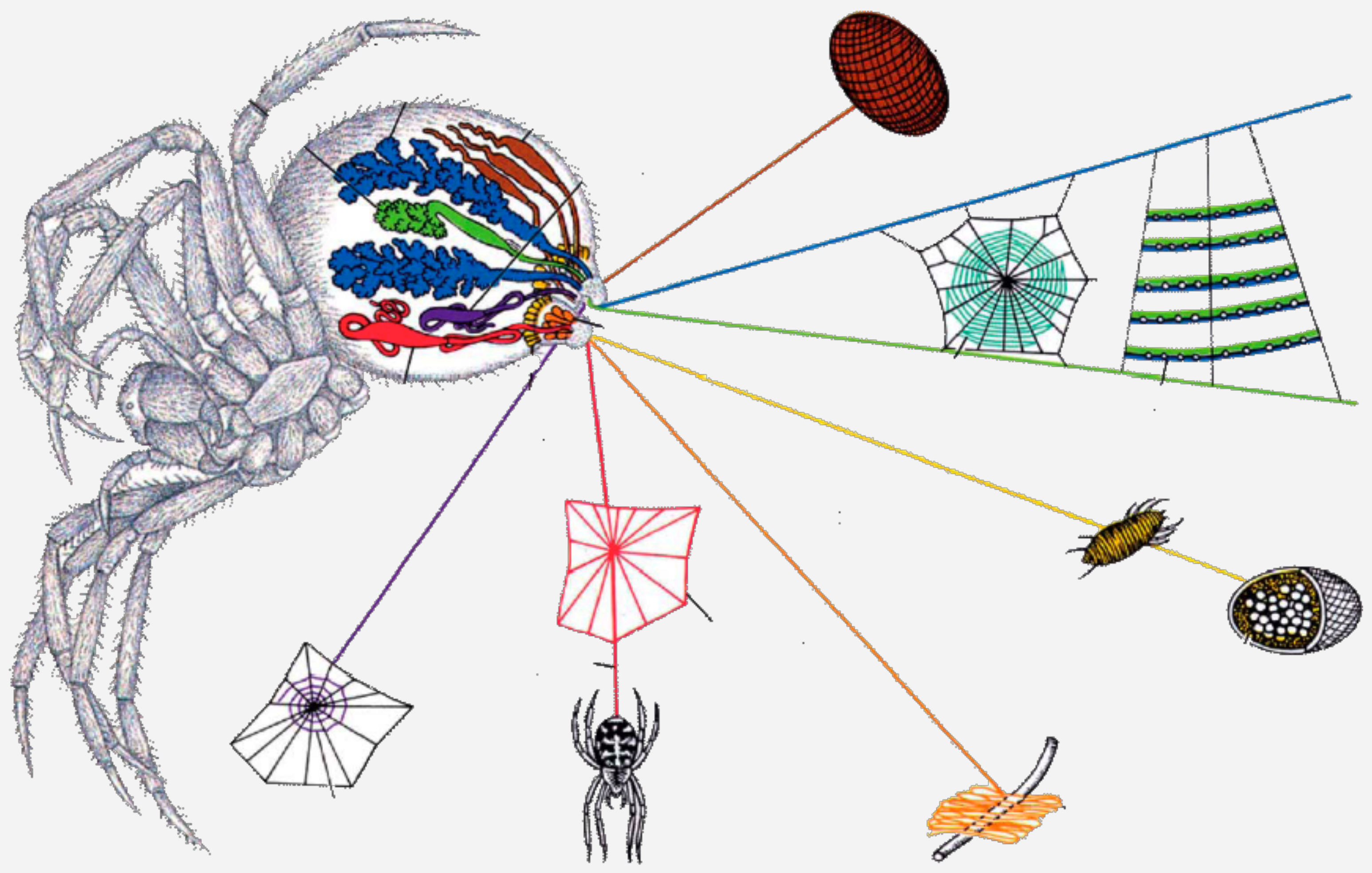
  geometric shape of the protein as result of supramolecular interactions between the amino acid side chains (hydrogen bonds, S–S bonds, electrostatic and van der Waals interactions)

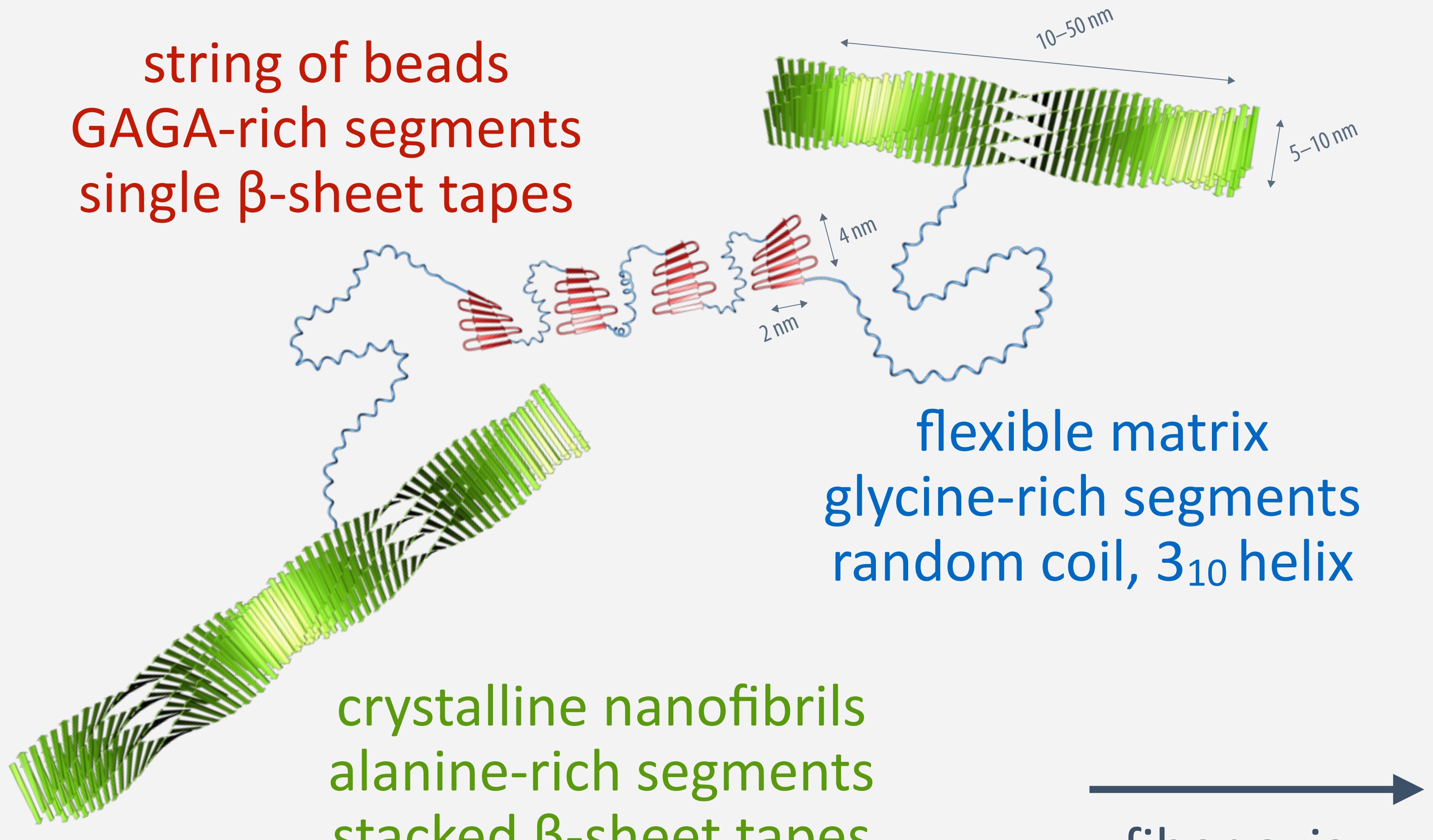
- **Quaternary Structure**

  aggregation of multiple proteins into multi-unit complex

- **proteins are defined macromolecules formed by concatenation of amino acid repeat units**

Nanostructure and Properties of Spider Dragline Silk





Material	Strength σ_{max} / GPa	Toughness 10^3 kJ m^{-1}	Stiffness GPa	Energy at Break kJ kg^{-1}	Extensibility ε_{max} / %
Spider Silk	1.1	160	10	100	27
Nylon	1	80		15	18
Kevlar	3.6	50	100	30	3
Steel	1.5	6	200	1	1
Rubber			0.001	10	1000

- **spider silk's high specific toughness due to hierarchical structures on different length scales**

The Role of Organic Chemistry for Technology

oil industry

→

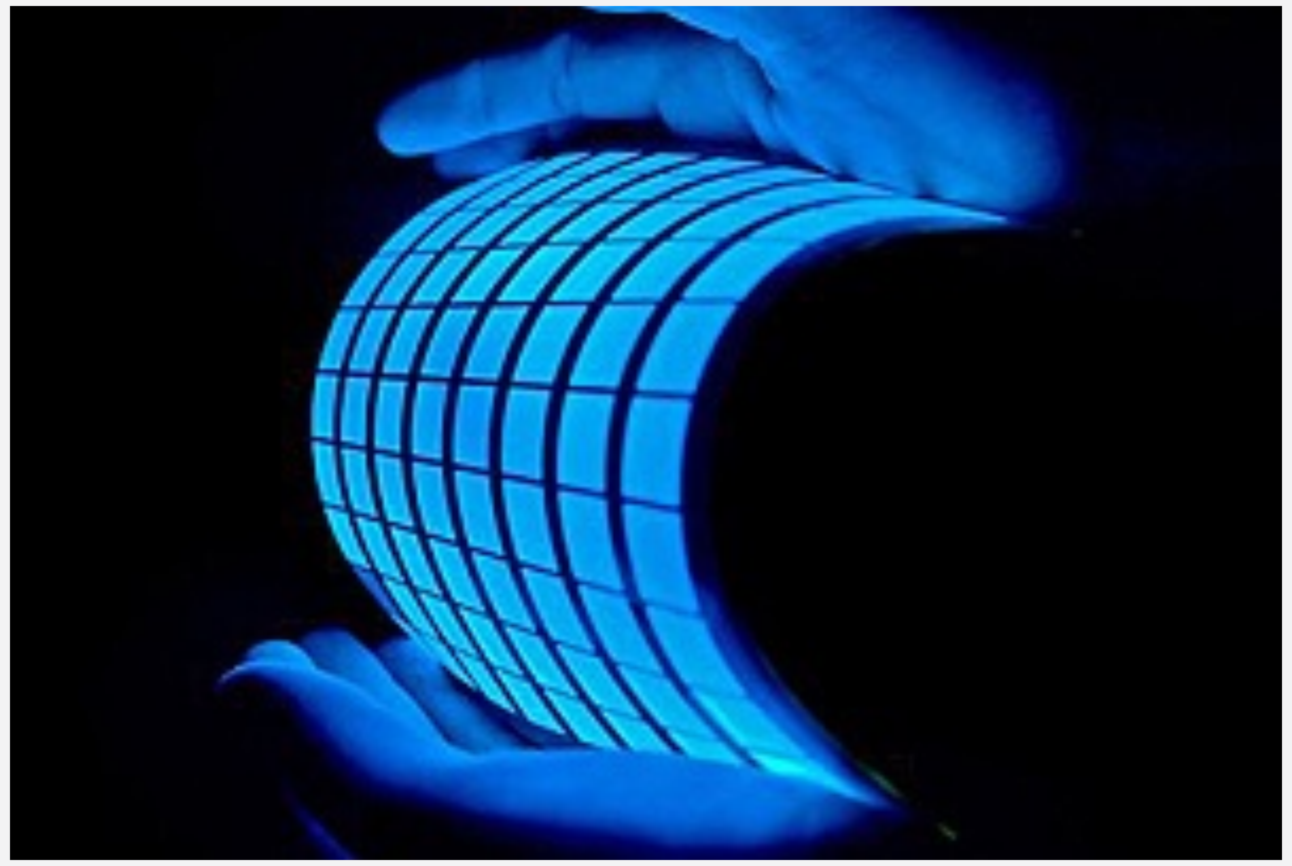
refinery industry

→

base and fine chemicals

crop protection

pharmaceutics



new materials

Polymer Materials & Sustainability

Polymer Science

bio-based

fossil-based

Natural Polymers | **Semi-Synthetic Polymers** | **Synthetic Polymers**

1922 Definition of the term "polymer" by Hermann Staudinger

1953 Nobel Prize for Hermann Staudinger (concept)

1963 Nobel Prize for Karl Ziegler and Giulio Natta (olefin polymerization)

1974 Nobel Prize for Paul J. Flory (polymers in solution)

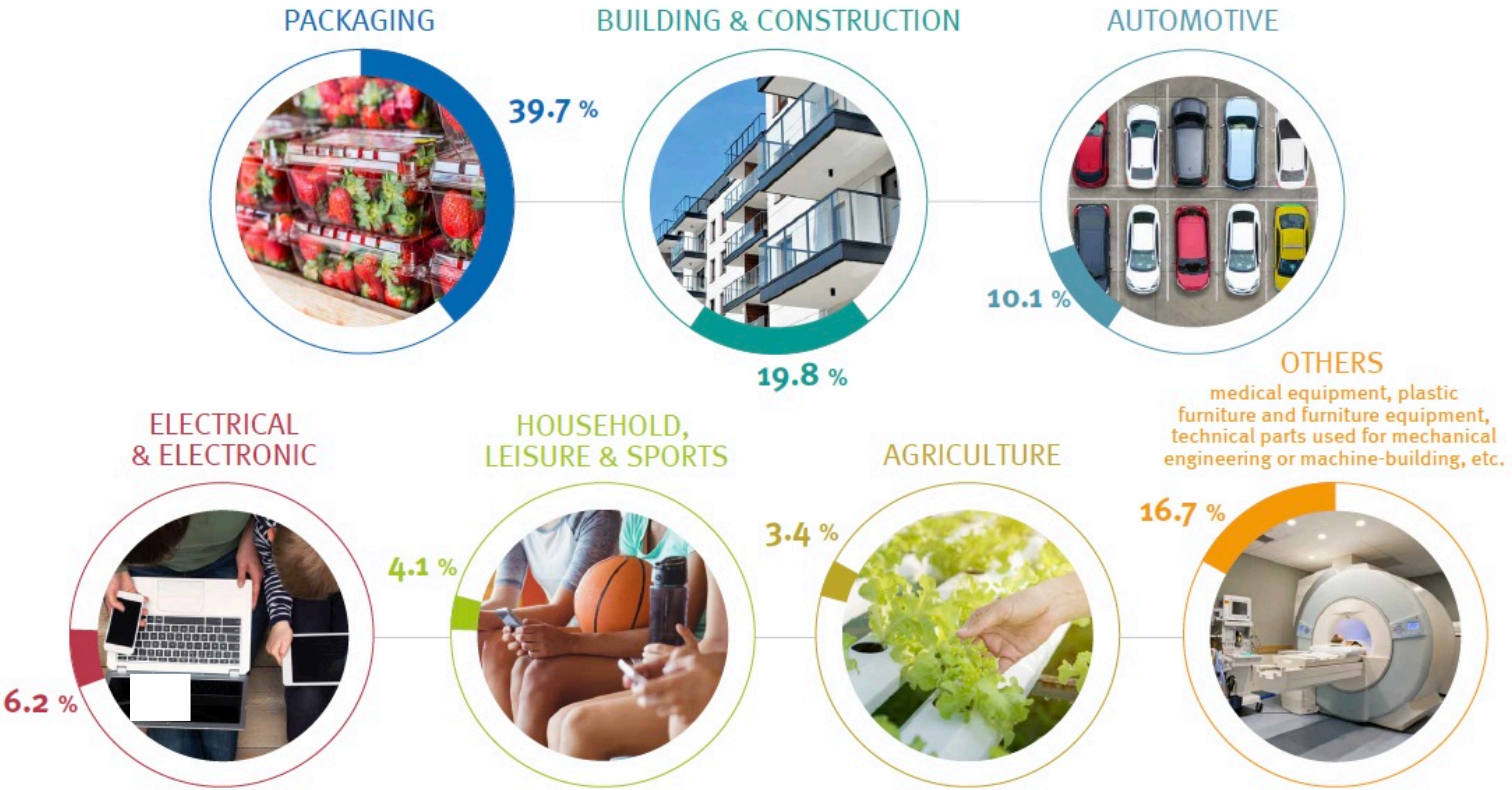
1991 Nobel Prize for deGennes (phase transitions)

2000 Nobel Prize for Heeger, MacDiarmid, Shirakawa (conductive polymers)

2005 Nobel Prize for Grubbs, Schrock, Chauvin (Olefin Methathesis)

Mühlhaupt, *Angew. Chem. Int. Ed.* **2004**, *43*, 1054.

Major Applications of Plastics



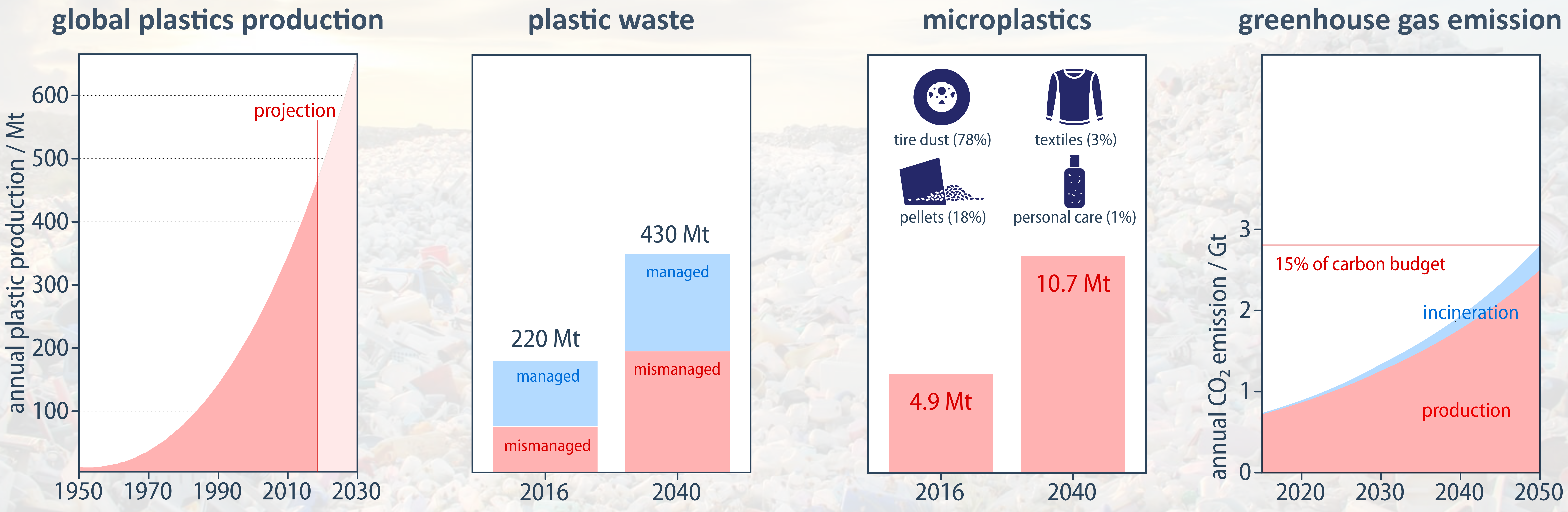
Sustainability Challenges of the Plastics Industry

- **This is not a regular landfill but the Thilafushi waste disposal site, a beach on the Maldives !**

Image © Mohamed Abdulraheem

Sustainability Challenges of the Plastics Industry

- continued plastics proliferation driven by low cost, light weight, performance, durability, design freedom
- plastics production doubles every 15 years, has produced 6.3 billion tons of plastic waste to date

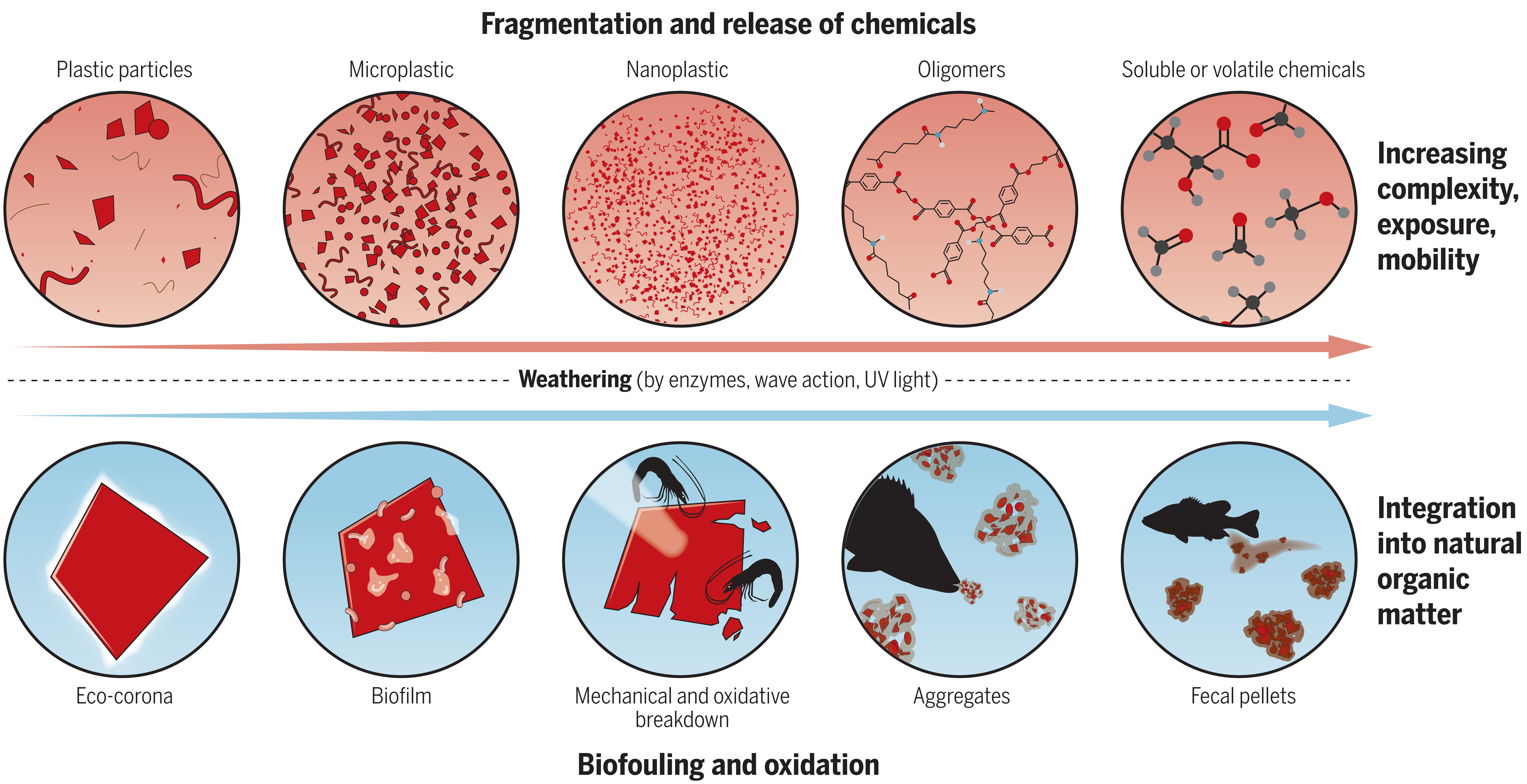


- **plastic waste and microplastics pollution are among the most serious challenges faced by mankind**
- **linear produce-use-discard model needs to be transfomed into a circular plastics economy**

Heinrich-Böll-Stiftung, *Plastikatlas*, **2019**; The Pew Charitable Trust & SYSTEMIQ, *Breaking the Plastic Wave*, **2020**; CIEL, *Plastic & Climate*, **2019**.

Awareness for the Plastic Waste Crisis Is Growing

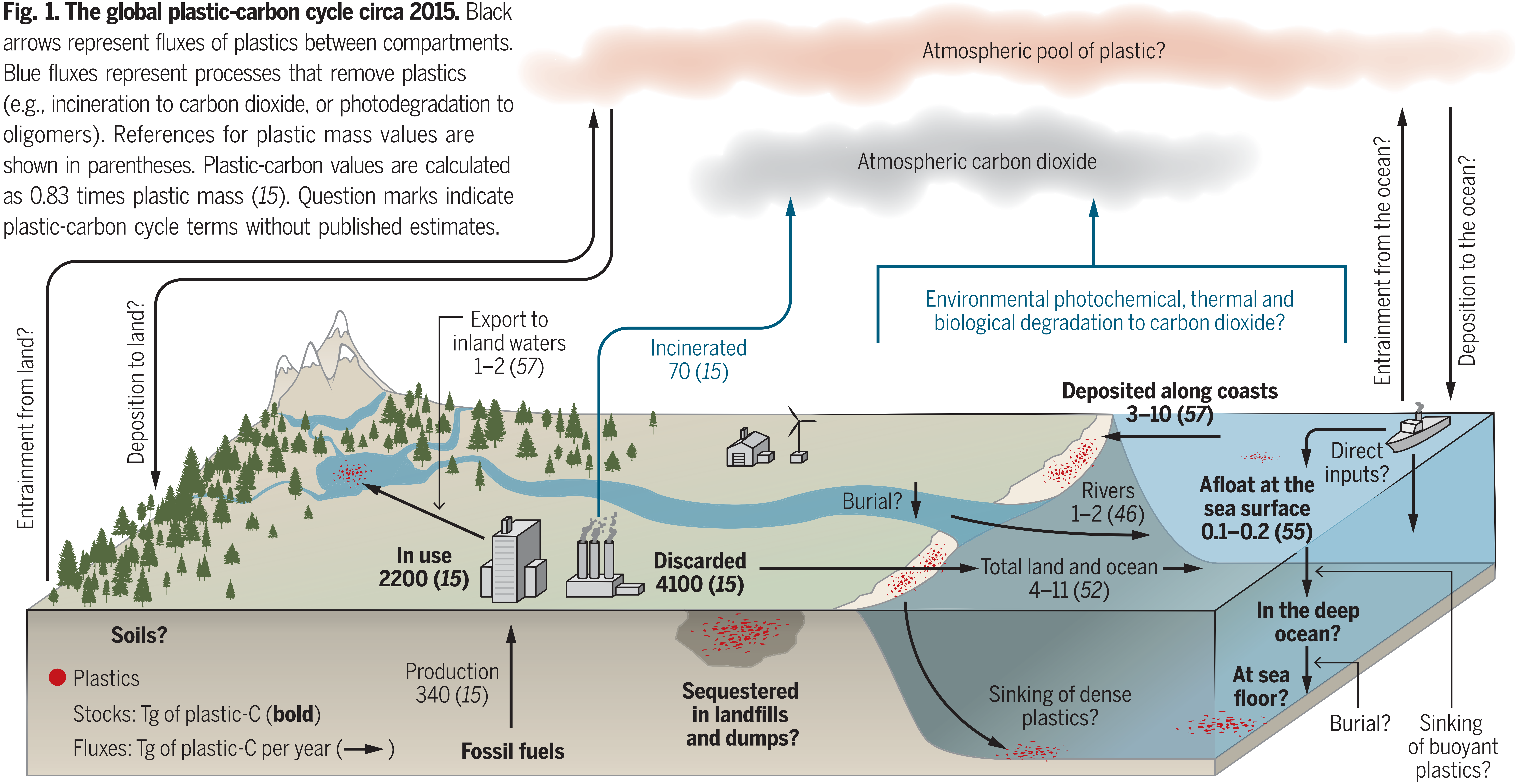
Plastics Weathering and Degradation



MacLeod et al., *Science* **2021**, *373 (6550)*, 61–65.

Plastics in The Earth System

Fig. 1. The global plastic-carbon cycle circa 2015. Black arrows represent fluxes of plastics between compartments. Blue fluxes represent processes that remove plastics (e.g., incineration to carbon dioxide, or photodegradation to oligomers). References for plastic mass values are shown in parentheses. Plastic-carbon values are calculated as 0.83 times plastic mass (*15*). Question marks indicate plastic-carbon cycle terms without published estimates.



Stubbins et al., *Science* **2021**, *373 (6550)*, 51–55

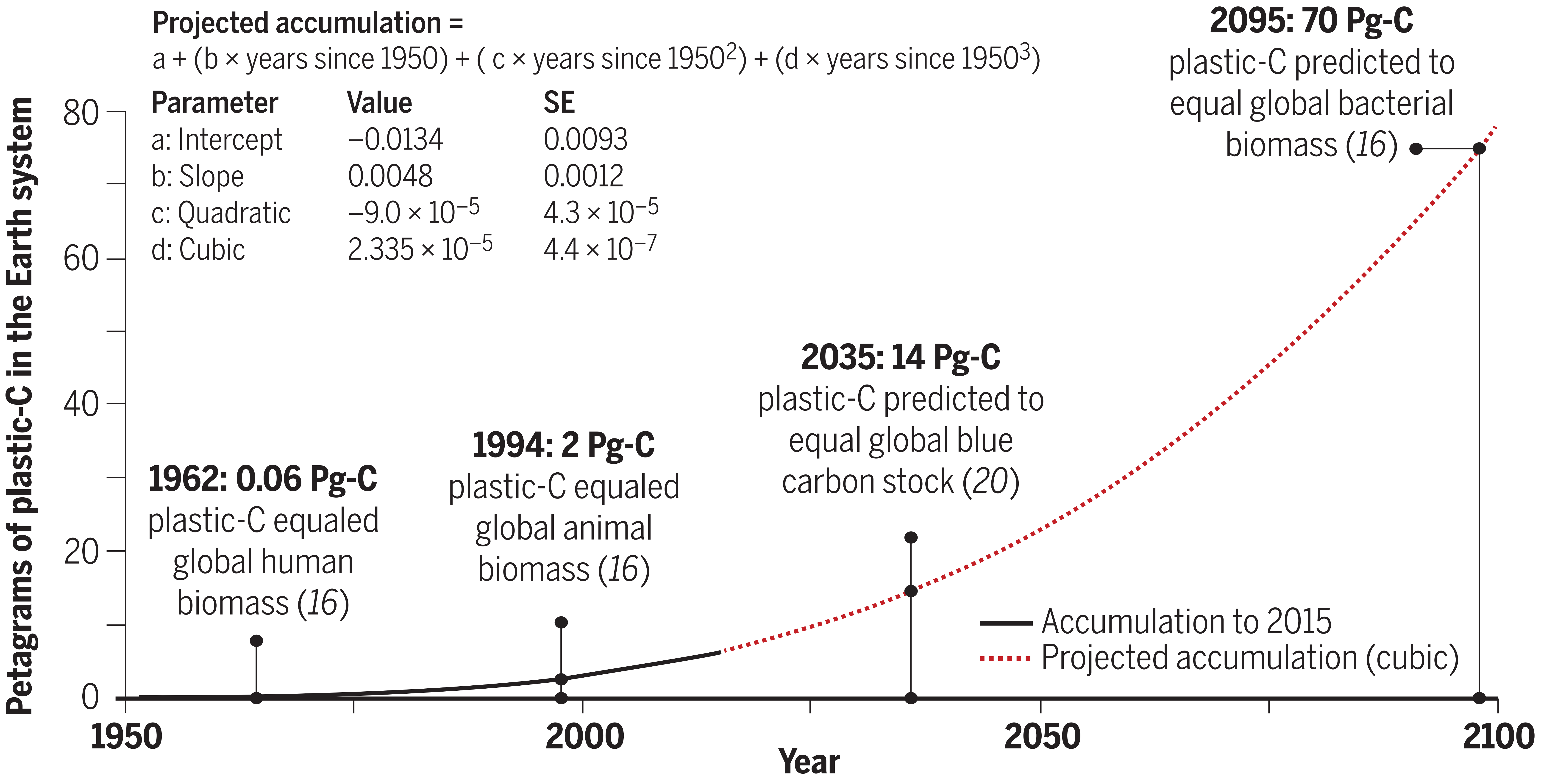


Fig. 3. Accumulation of plastic-carbon in the Earth system. Accumulation of plastic up to 2015 calculated as production minus incineration (*15*). Projected accumulation calculated assuming current trend (cubic growth) for plastic accumulation will continue into the future. The cubic model had the lowest Akaike information criterion of models in JMP. Actual future plastic-carbon accumulation will depend on hard-to-predict socioeconomic factors. Biomass numbers refer to living biomass.

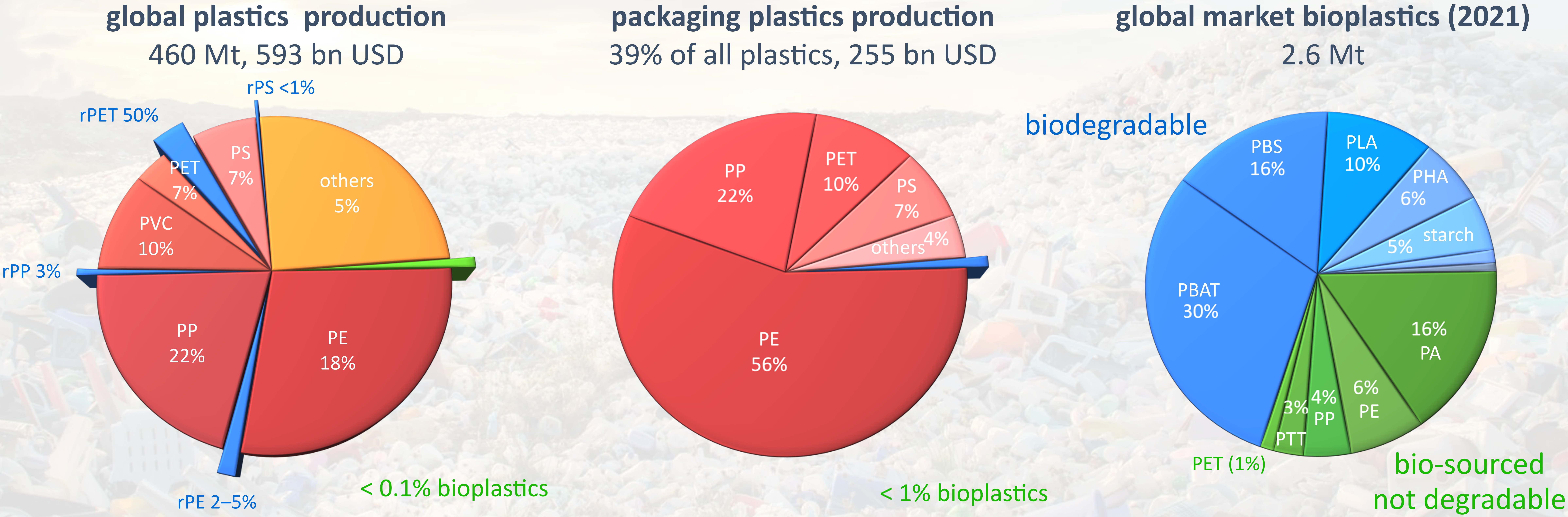
Plastics Production, Waste, and Pollution

- **plastics production keeps growing, follows a linear value chain paradigm**
  - global production 335 Mt in 2016, 60 Mt in Europe
  - 40% for packaging, will double until 2034
- **plastics waste & pollution are major socioeconomic challenges**
  - global recycling rate stagnates at 14%
  - 40% ends up in landfill,10% enters the ocean
- **microplastics pollution is a global environmental desaster**
  - atmospheric transport to remote areas
  - infiltration of the entire food chain
  - a solution requires a rethinking of the recycling system and economy

Nature Geoscience **2019**, *12*, 339; *Plastik Atlas* **2019**.

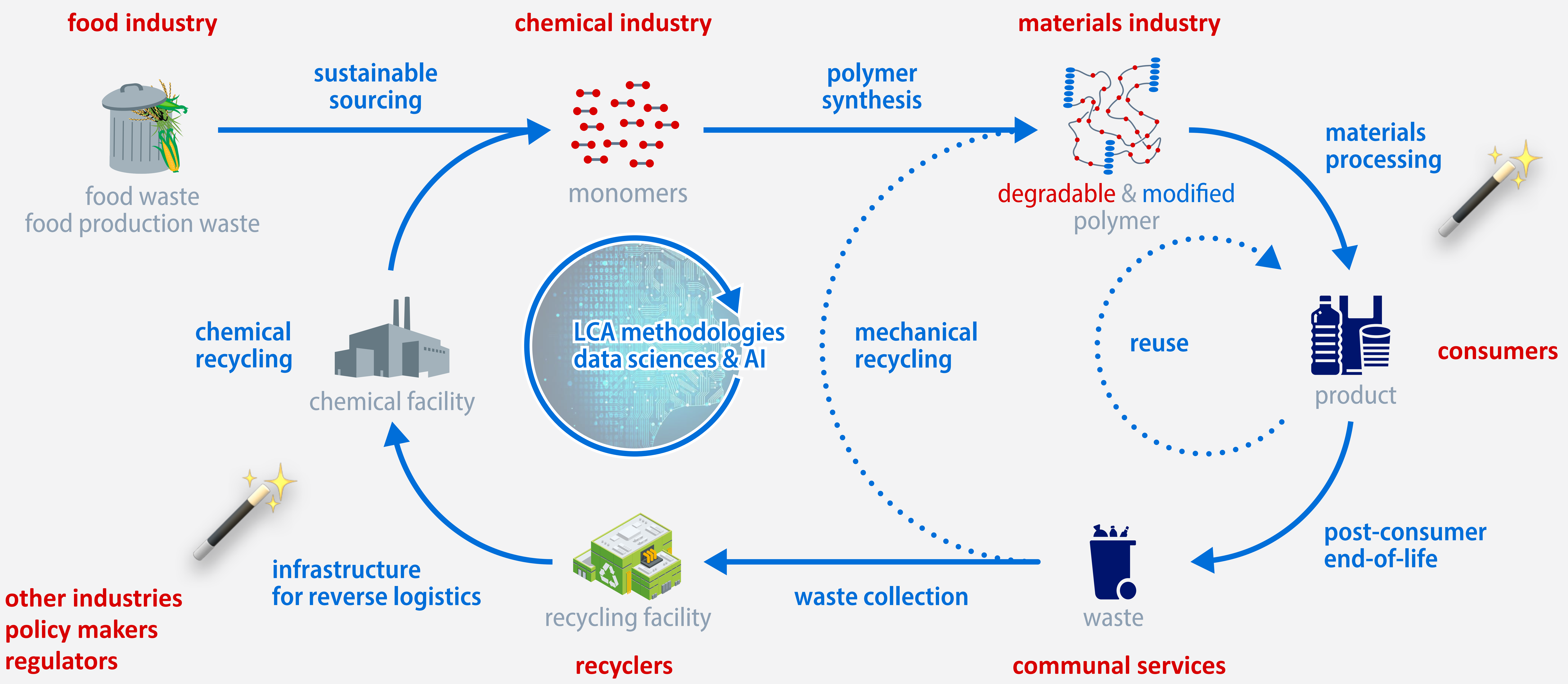
Current Commodity Plastics and Recycling

- EU Legislation: all packaging plastic reusable or recyclable by 2030 ! Reduce, Reuse, Recycle !
- efficient recovery, sorting, separation and recycling require reduced set grades, components



- **Challenge: reduced set of polymer materials and components must be adapted to the broad range of processing requirements and final product performance solutions they are intended to replace !**

Systems View of the Circular Plastics Economy

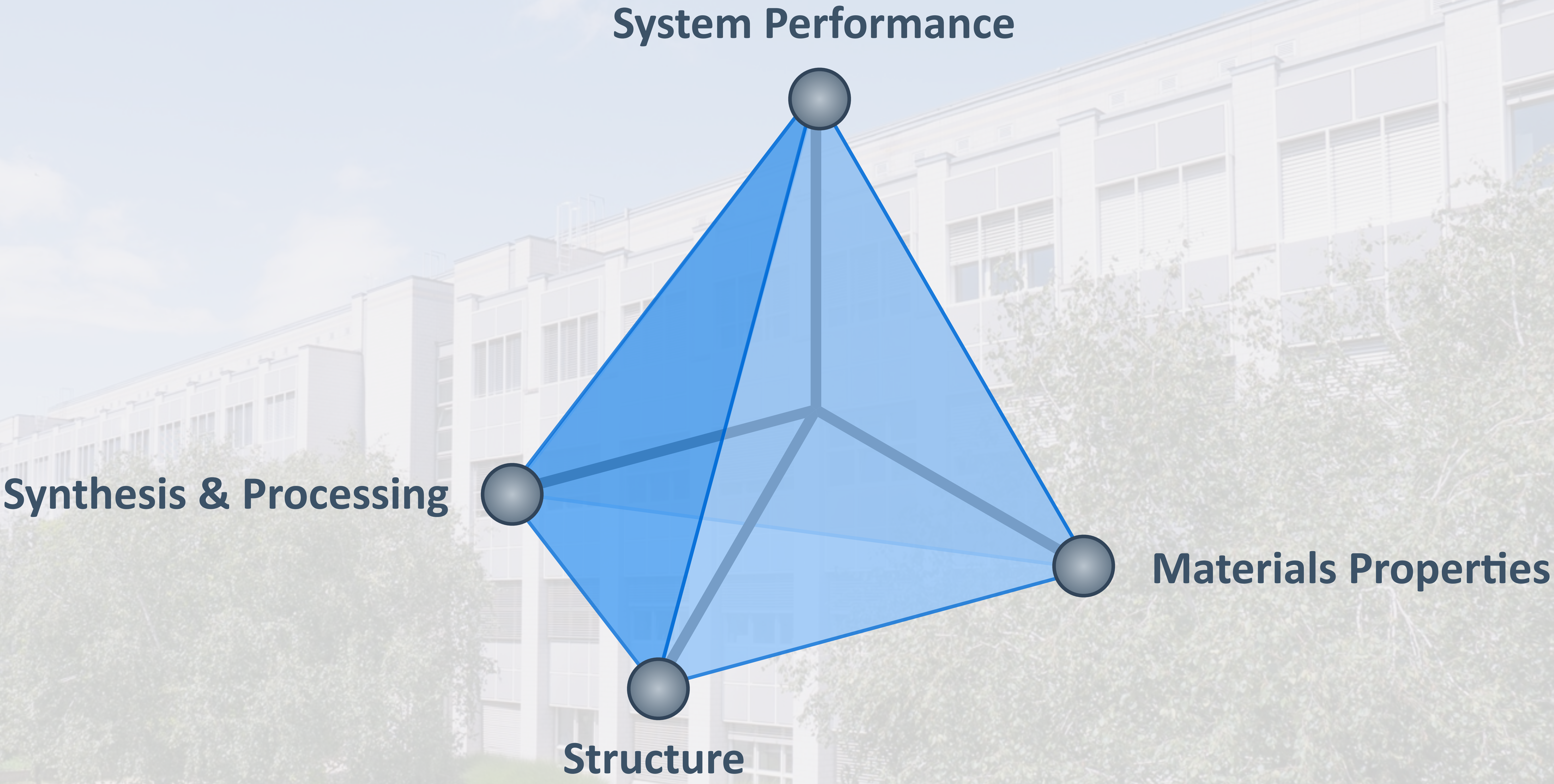


- addressing the plastic waste crisis requires changes at systems level involving many stakeholders

Polymers & Soft Matter at the Institute of Materials

“Everything is Made of Something”

- materials science is in many ways a foundational discipline for all other fields of science & engineering

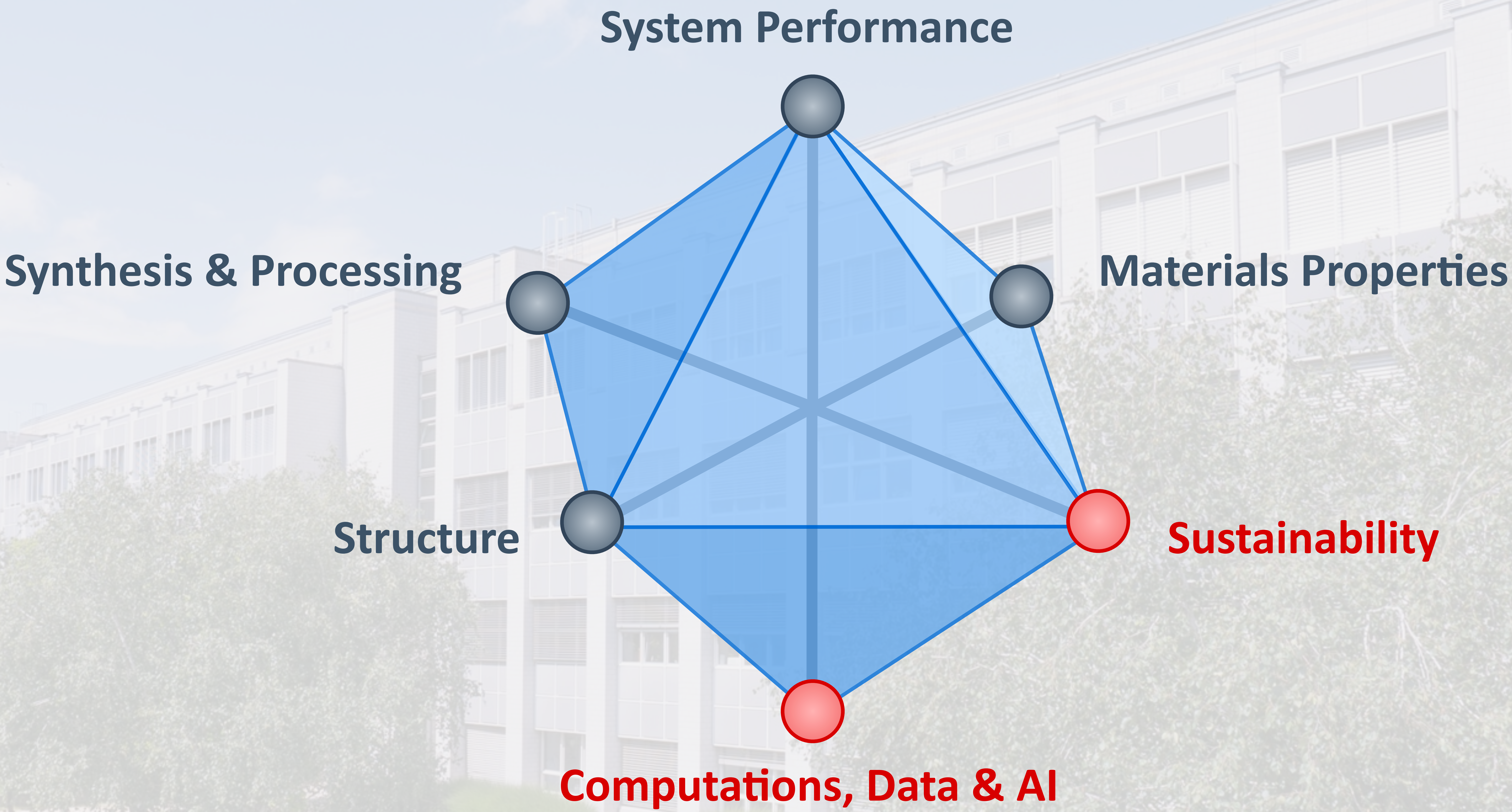


- **diversity and interdisciplinarity are inherent and paramount to the field of materials science, which is also populated by researchers from physics, chemistry, biology, and engineering**

Ashby, Shercliff, Cebon, *Materials: Engineering, Science, Processing and Design*, Elsevier, **2018**.

The Future of Materials Science

- materials science is evolving and needs to respond to societal and technological challenges

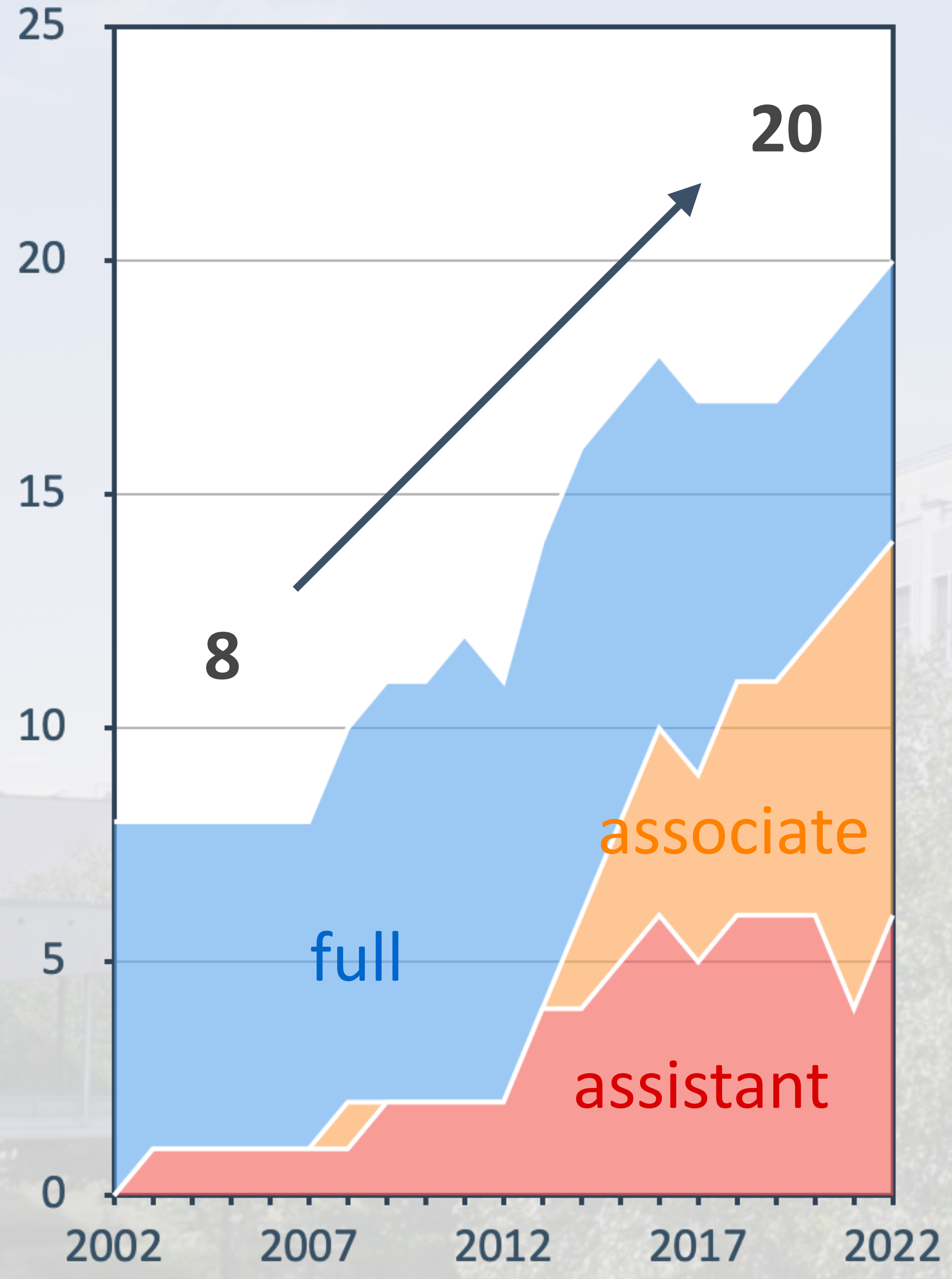


- **our vision of the future of materials science emphasizes the convergence of synthetic & biological worlds, and in particular the major role of sustainability and digital technologies**

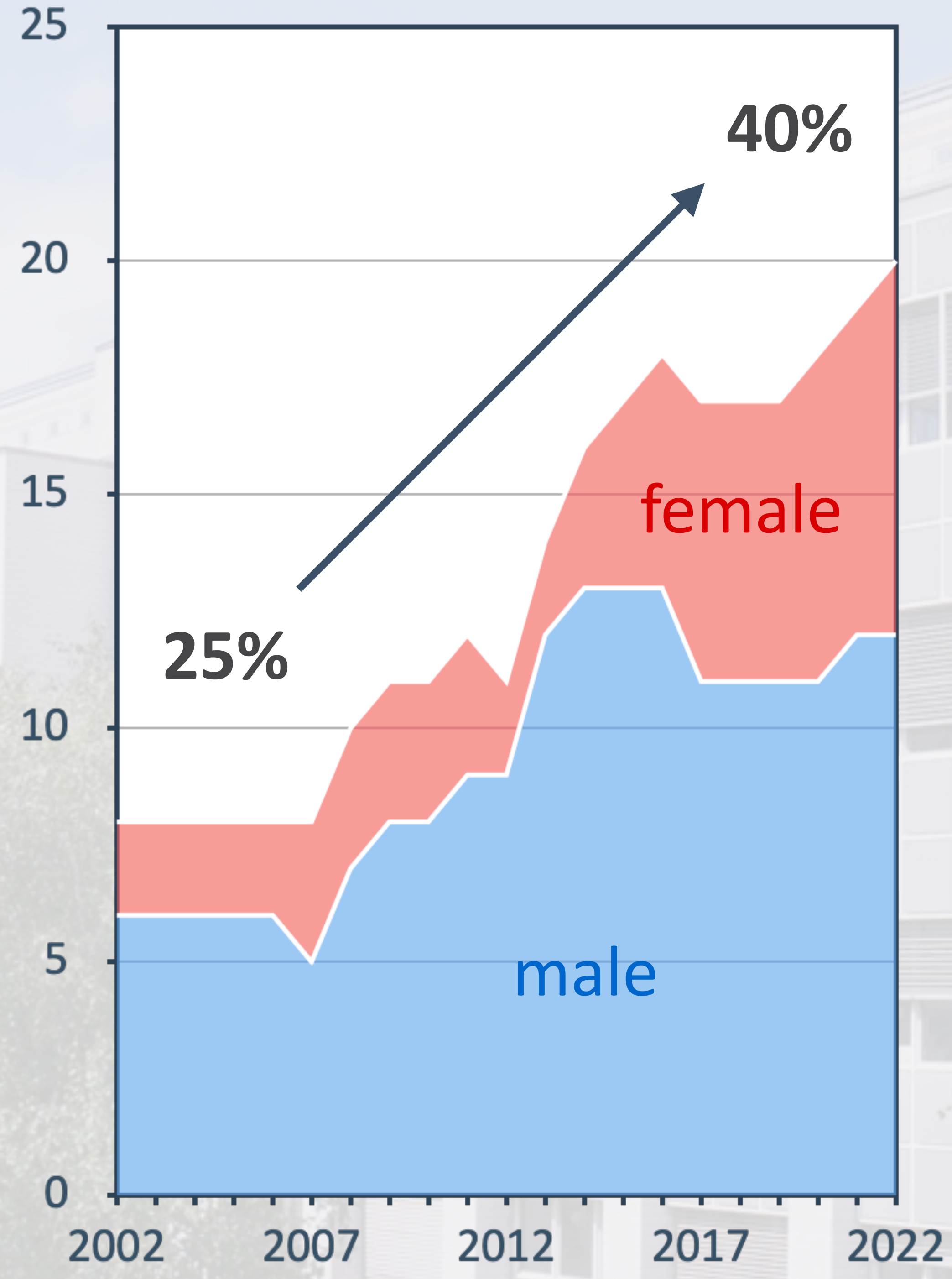
EPFL Institute of Materials

- materials science at EPFL is a diverse, well-balanced and thriving scientific community !

Faculty



Faculty Gender Balance



QS World University Rankings 2023 Materials Science

1	Massachussetts Institute of Technology	USA
2	Stanford University	USA
3	University of Cambridge	UK
4	Harvard University	UK
5	University of California, Berkeley (UCB)	USA
6	Nanyang Technological University, Singapore (NTU)	Singapore
7	University of Oxford	UK
8	**EPFL**	**CH**
9	Imperial College London	UK
10	Tsinghua University	China
11	ETH Zurich	CH
12	National University of Singapore (NUS)	Singapore
13	Georgia Institute of Technology	USA
14	California Institute of Technology	USA
15	Northwestern University	USA

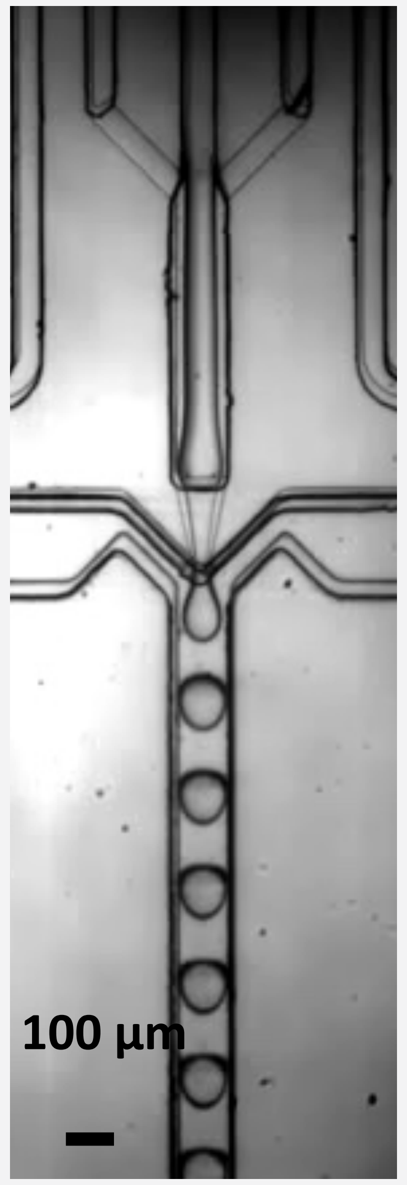
- **consistently ranking in the top 10 materials science departments since 2018 !**
- **world reputation in soft, construction, and quantum materials, as well as modeling & computations**

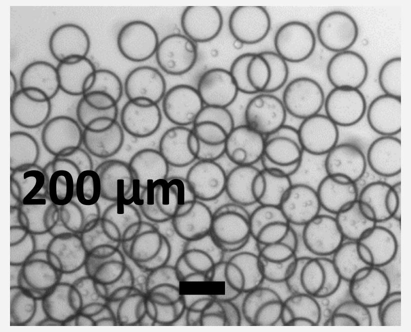
Soft Matter Activities at the Institute of Materials

Laboratory of Mechanical Metallurgy (LMM)	Andreas Mortensen
Laboratory of Construction Materials (LMC)	Karen Scrivener
Polymers Laboratory (LP)	Harm-Anton Klok
Tribology and Interfacial Chemistry Laboratory (TIC)	Stefano Mischler
Laboratory of Semiconductor Materials (LMSC)	Anna Fontcuberta
Laboratory of Organic and Macromolecular Materials (LMOM)	Holger Frauenrath
Supramolecular Nanomaterials & Interfaces Laboratory (SUNMIL)	Francesco Stellacci
Laboratory of Theory and Simulation of Materials (THEOS)	Nicola Marzari
Laboratory of Photonic Materials and Fibre Devices (FIMAP)	Fabien Sorin
Laboratory of Computational Science and Modelling (COSMO)	Michele Ceriotti
Laboratory of Thermomechanical Metallurgy (LMTM)	Roland Logé
Soft Materials Laboratory (SMAL)	Esther Amstad (PATT)
Laboratory of Nanoscale Magnetic Materials & Magnonics (LMGN)	Dirk Grundler
In Situ Nanomaterials Characterization with Electron (INE)	Vasiliki Tileli (PATT)
Laboratory for Processing of Advanced Composites (LPAC)	Véronique Michaud
Programmable Biomaterials Laboratory (PBL)	Maartje Bastings (PATT)
Laboratory for Sustainable Materials (SUMA)	Tiffany Abitbol (PATT)
Laboratory for X-ray Characterization of Materials (CAM-X)	Marianne Liebi (PATT)

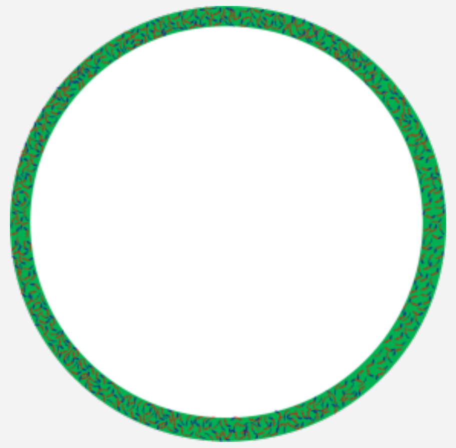
Soft Materials Laboratory (SMAL, Esther Amstad)

Capsules from Self-assembled Block Copolymers

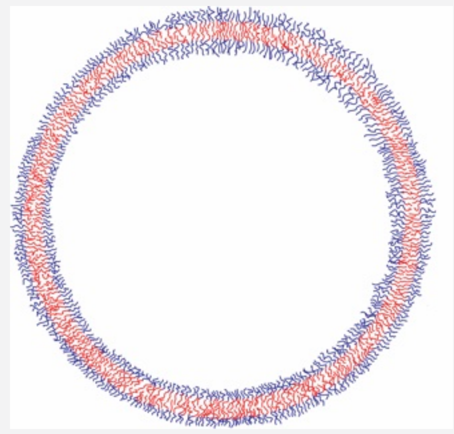




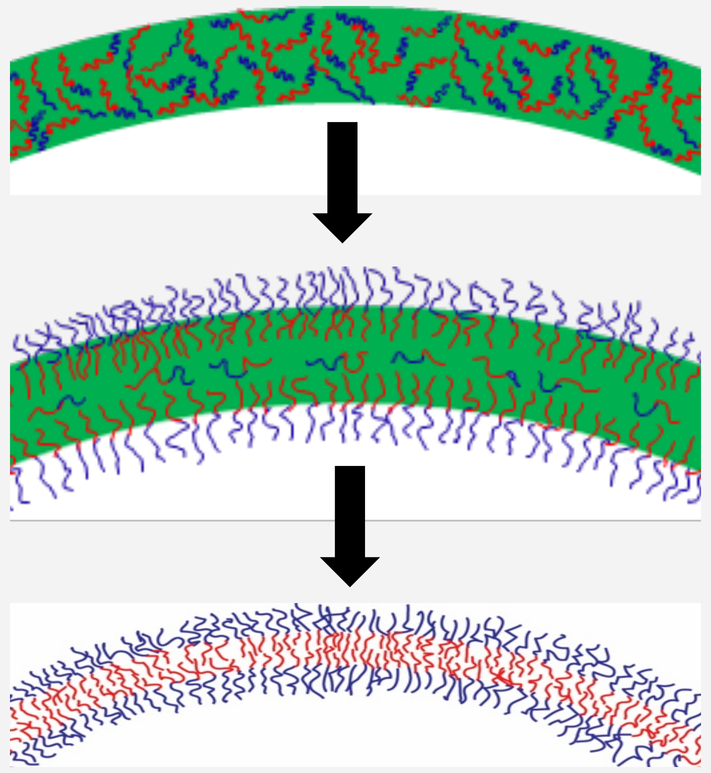
water/oil/water double emulsion



vesicle

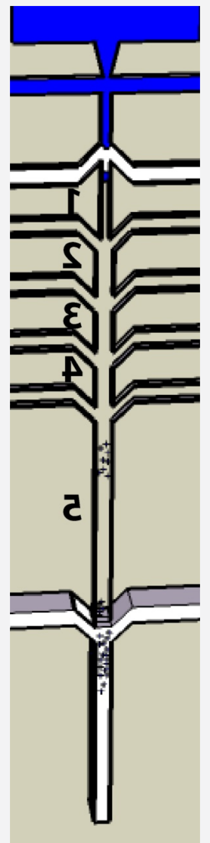


self-assembly upon drying

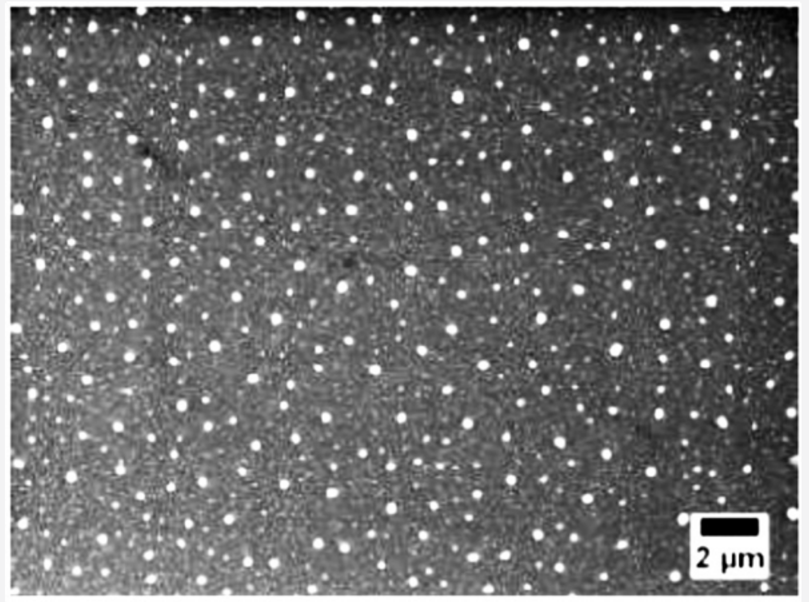


Early Stages of Crystallization

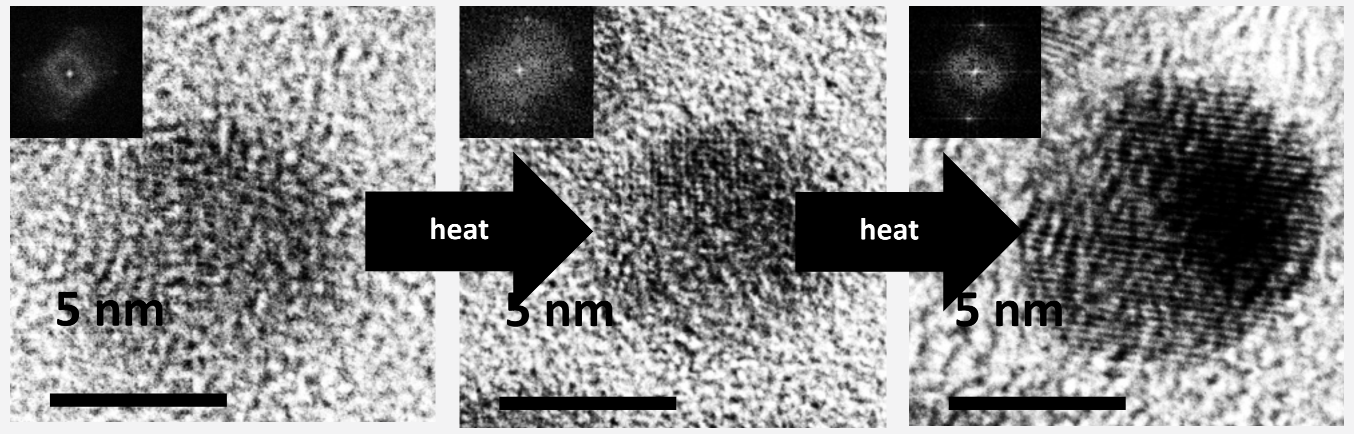
microfluidic spray drier



spray dried nanoparticles



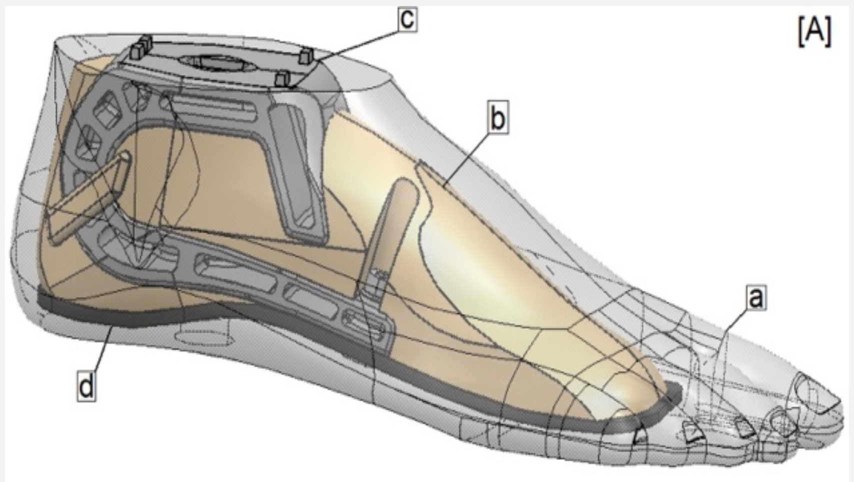
crystallization



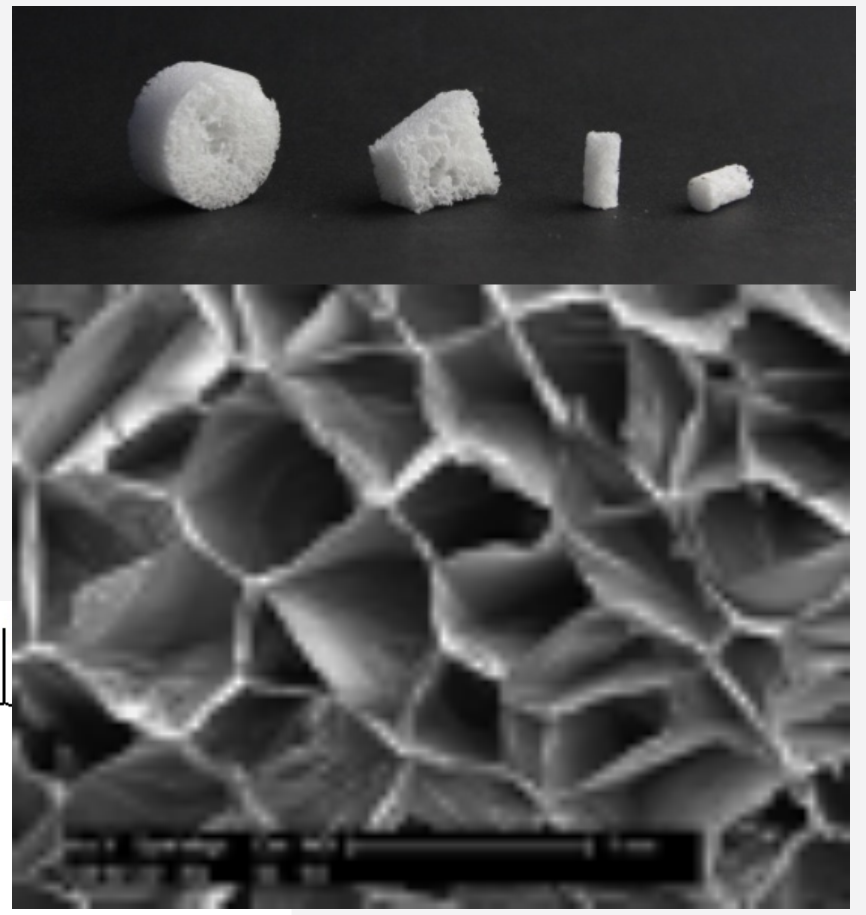
- **SMAL focuses on using polymers for compartmentalization and microstructure control**

Laboratory of Advanced Composites (LPAC, Veronique Michaud)

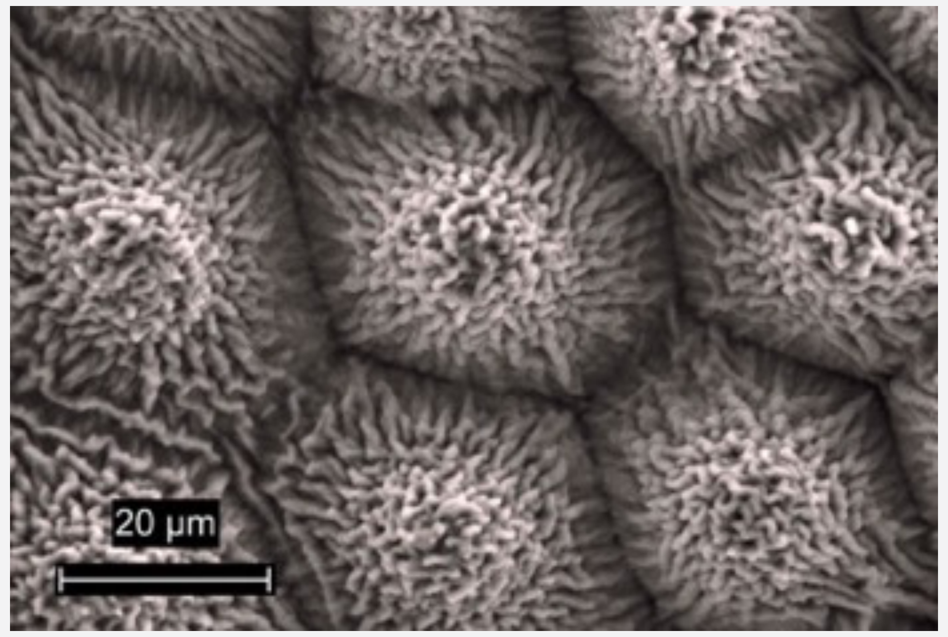
- LPAC focuses on the fundamentals of composite and hybrid materials processing

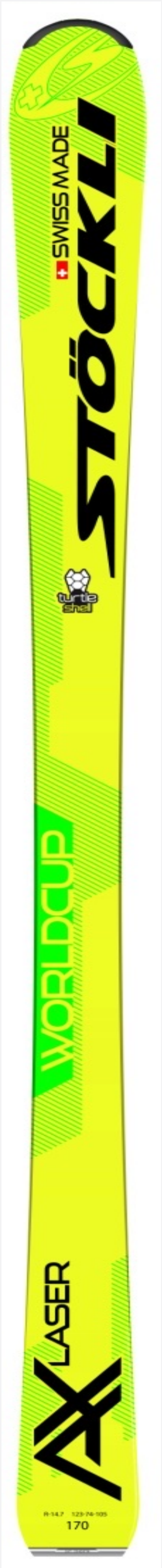


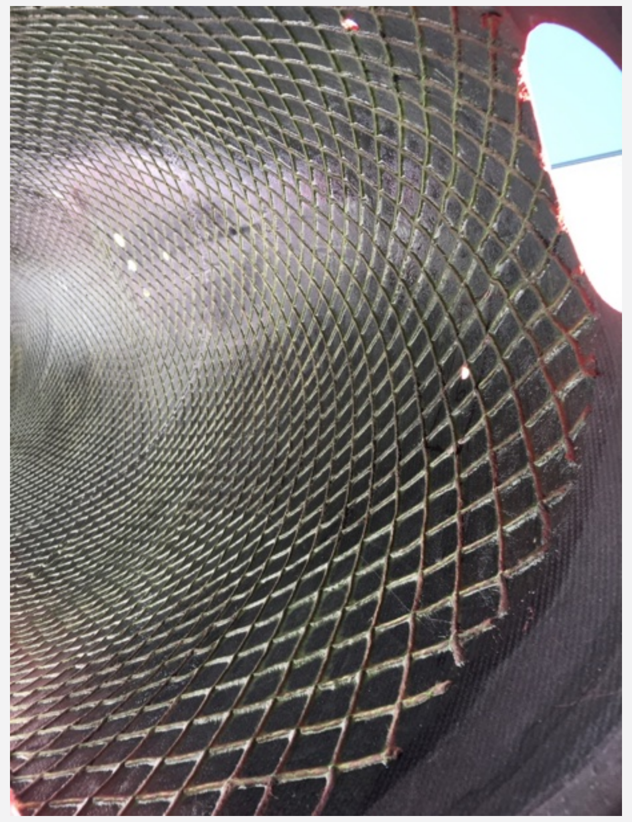
Biodegradable foams for medical applications



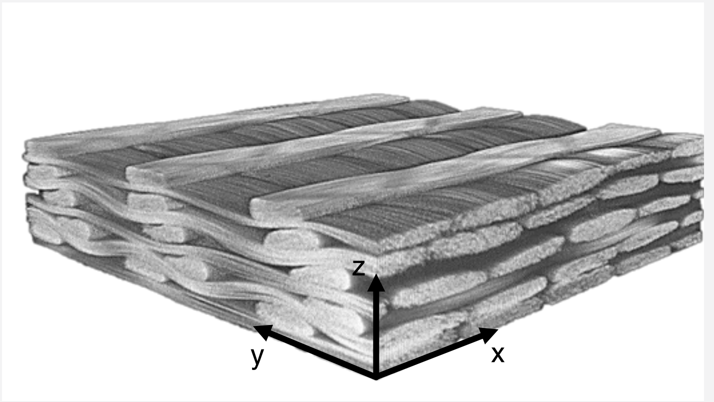
Bioinspired self-cleaning and wear-resistant surfaces



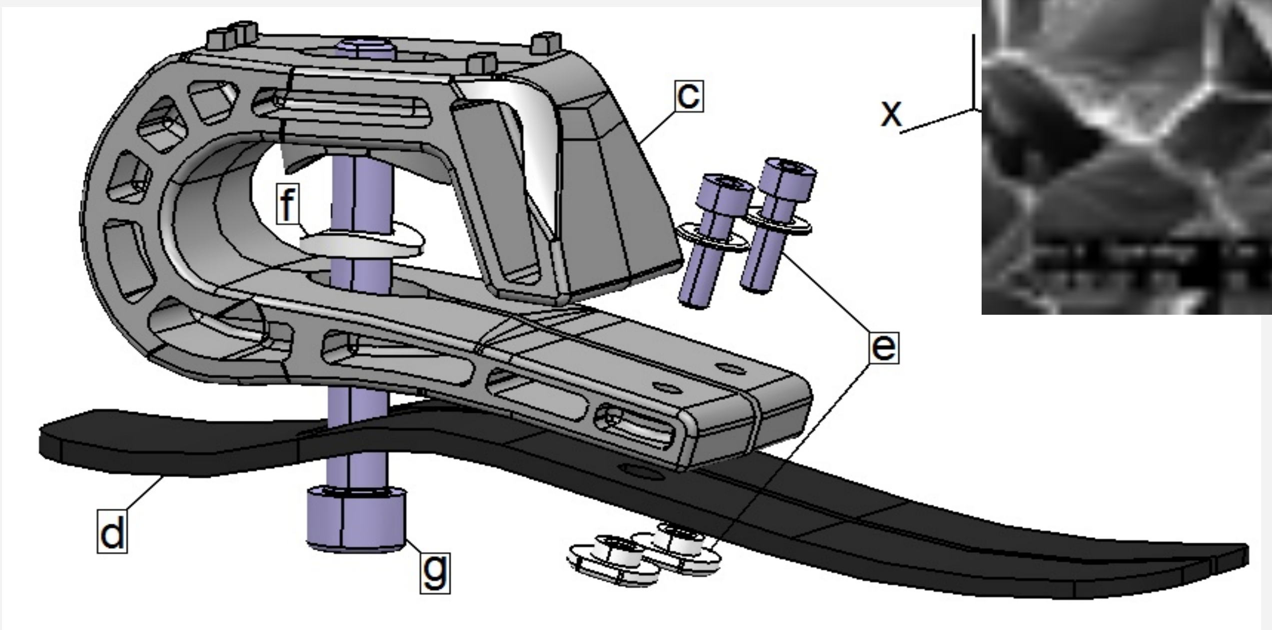




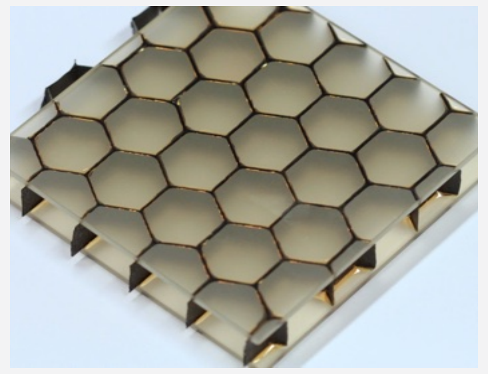
Flax Power Ribs (Bcomp)



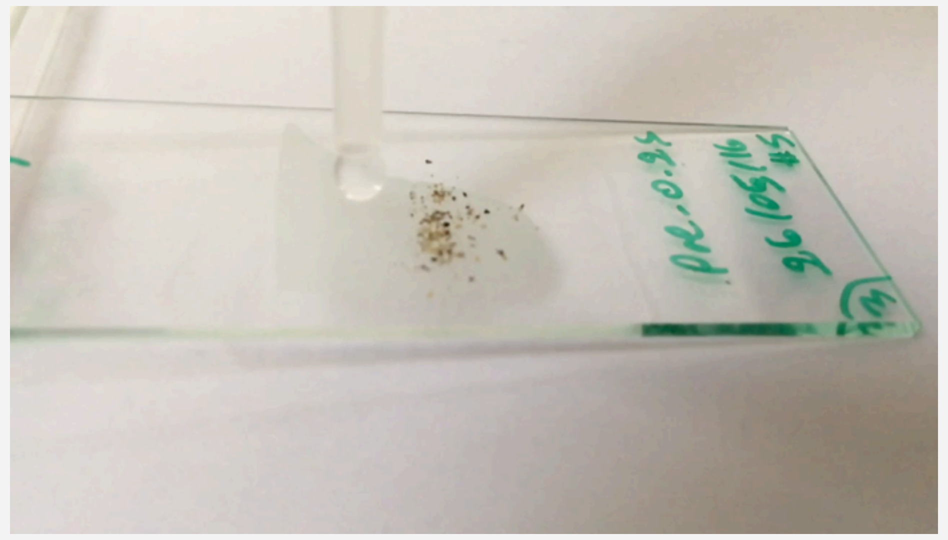
Textiles



Agilis project: composites, injection molded polymers, foams



Sandwiches

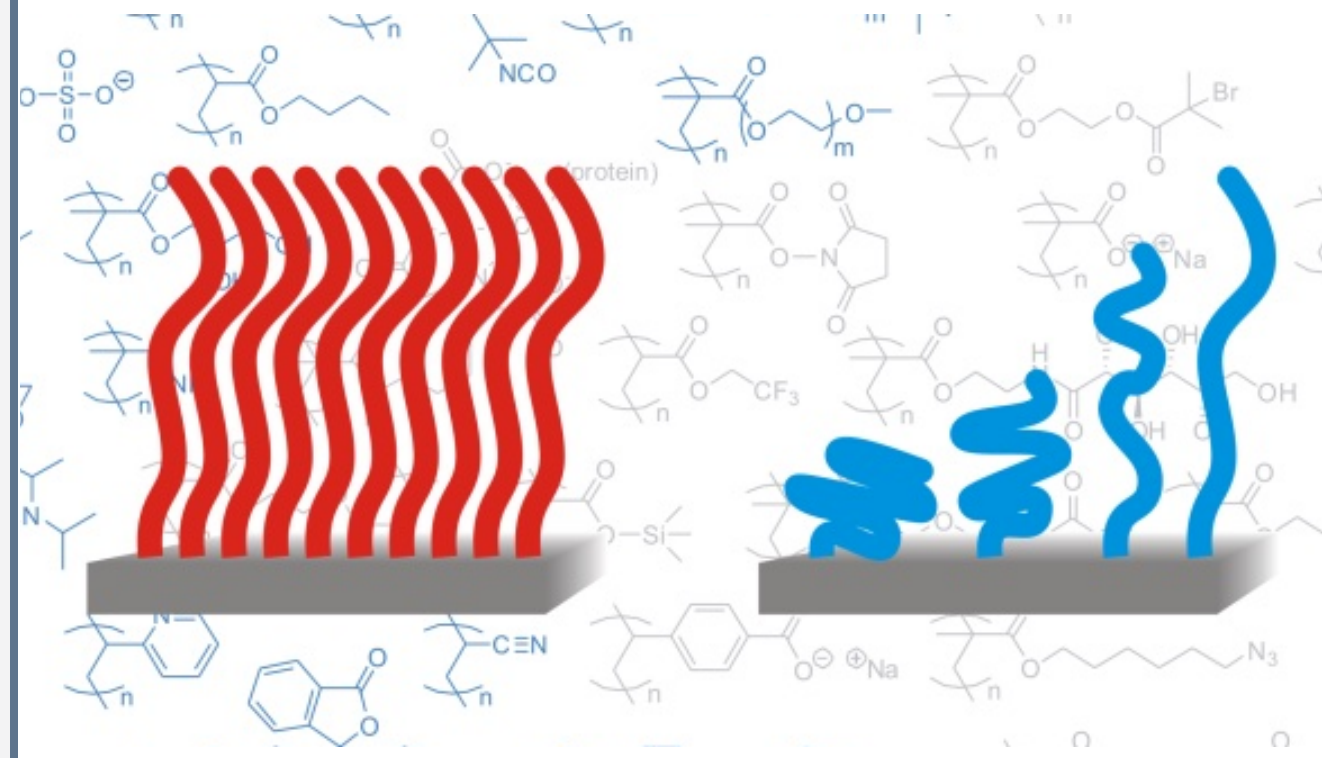


Synthetic yellow rose petal surface with pepper grains

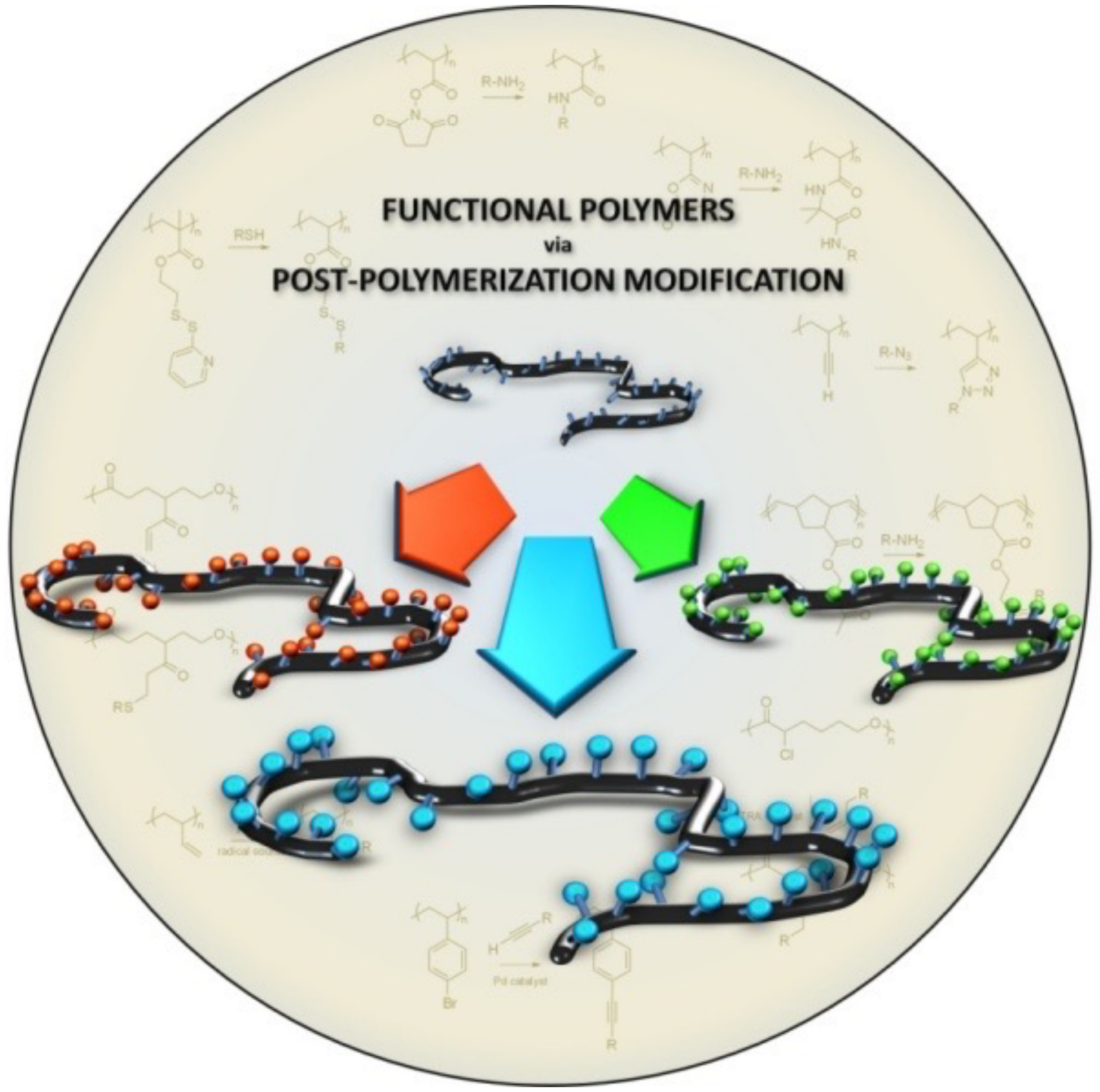
- **fundamentals of polymers and composite materials processing**
- **surface and interfaces (bioinspired surfaces, adhesion and bonding)**

Polymer Laboratory (LP, Harm-Anton Klok)

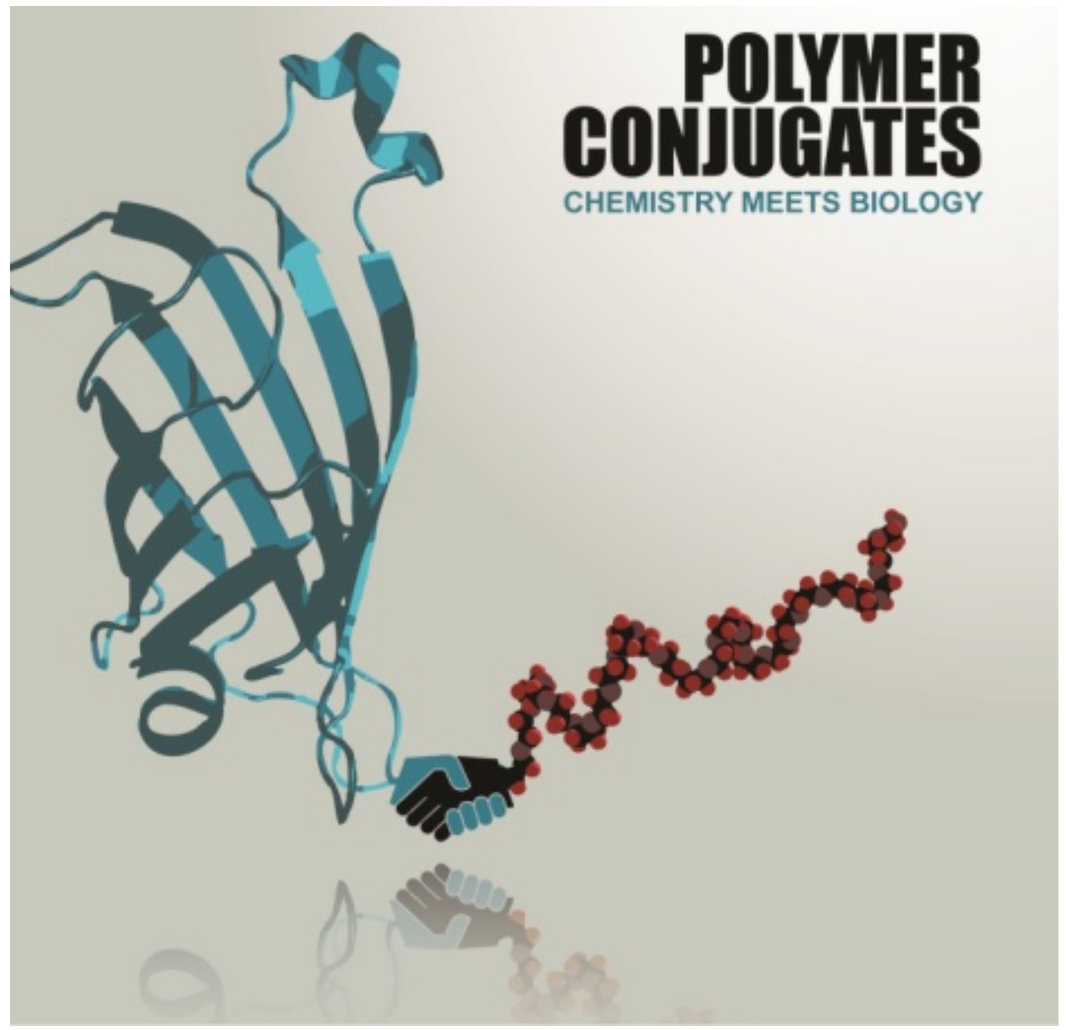
Polymer Surfaces & Interfaces



Precision Polymer Synthesis



Polymer Bioconjugates

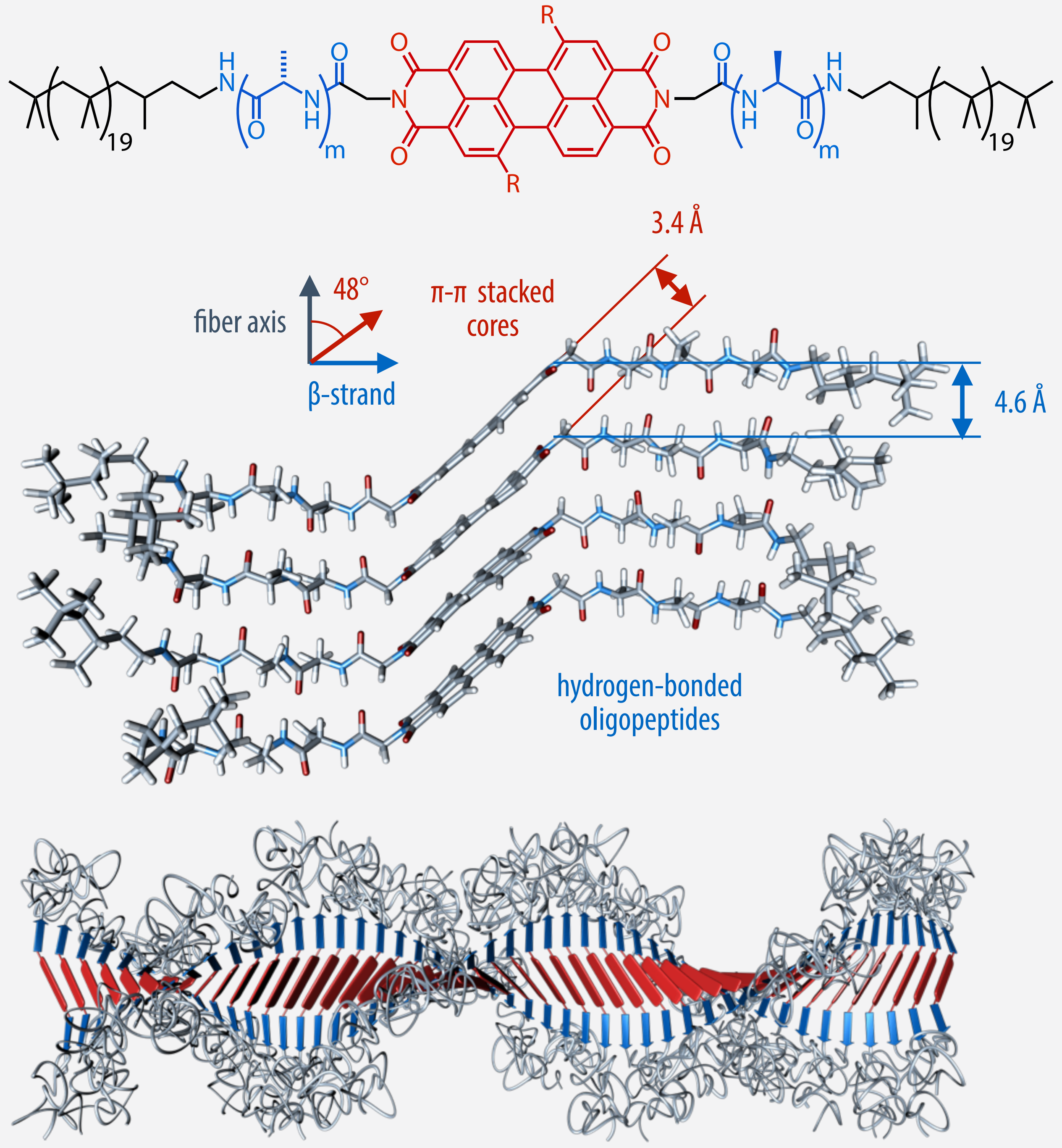


- peptide/protein-based polymer materials and hybrid materials for polymer therapeutics
- surface-initiated polymerization and polymer brushes for microarrays, chemical sensing

Laboratory of Macromolecular and Organic Materials

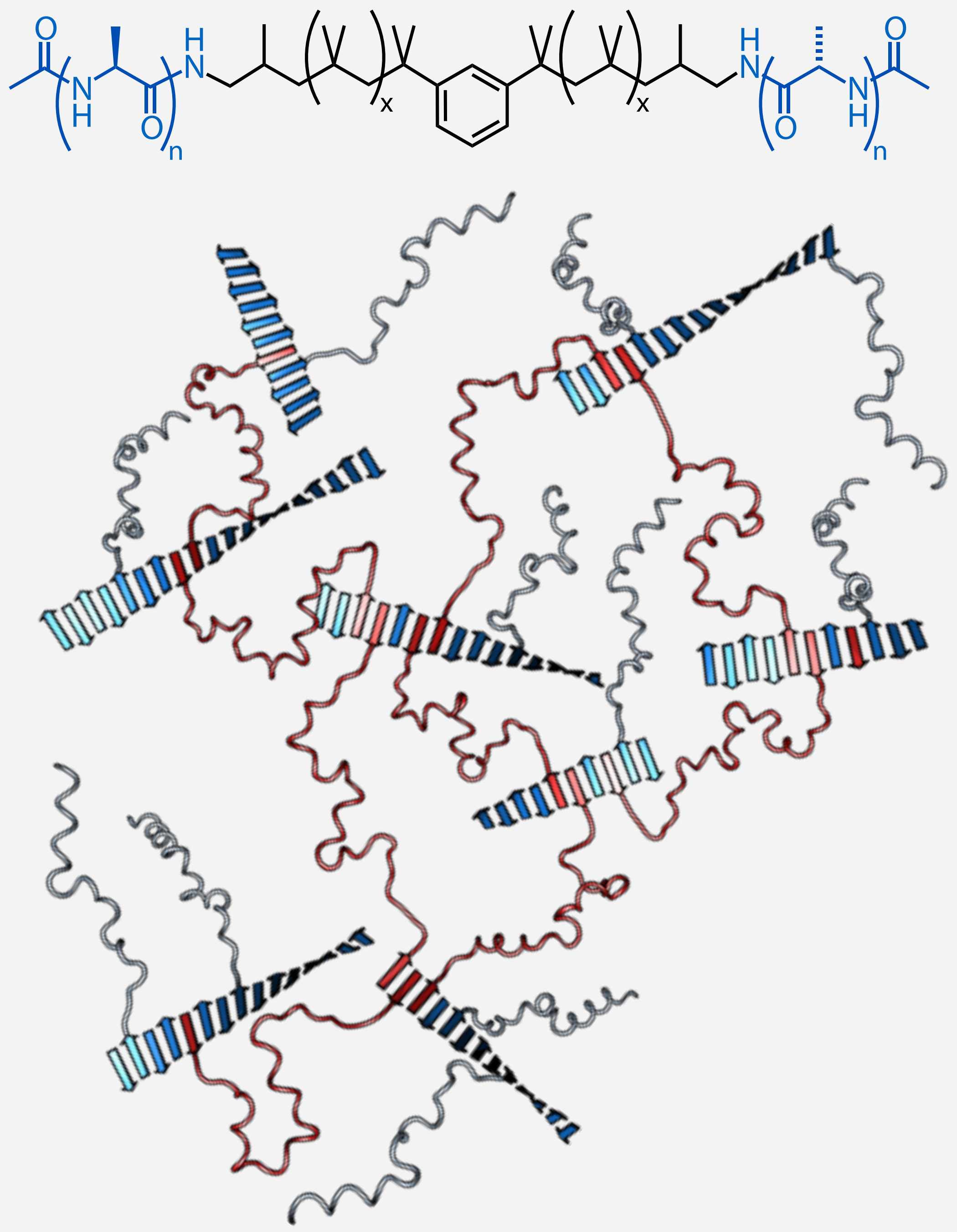
- **universal supramolecular approach** to control diverse functions in different materials classes

electronic properties



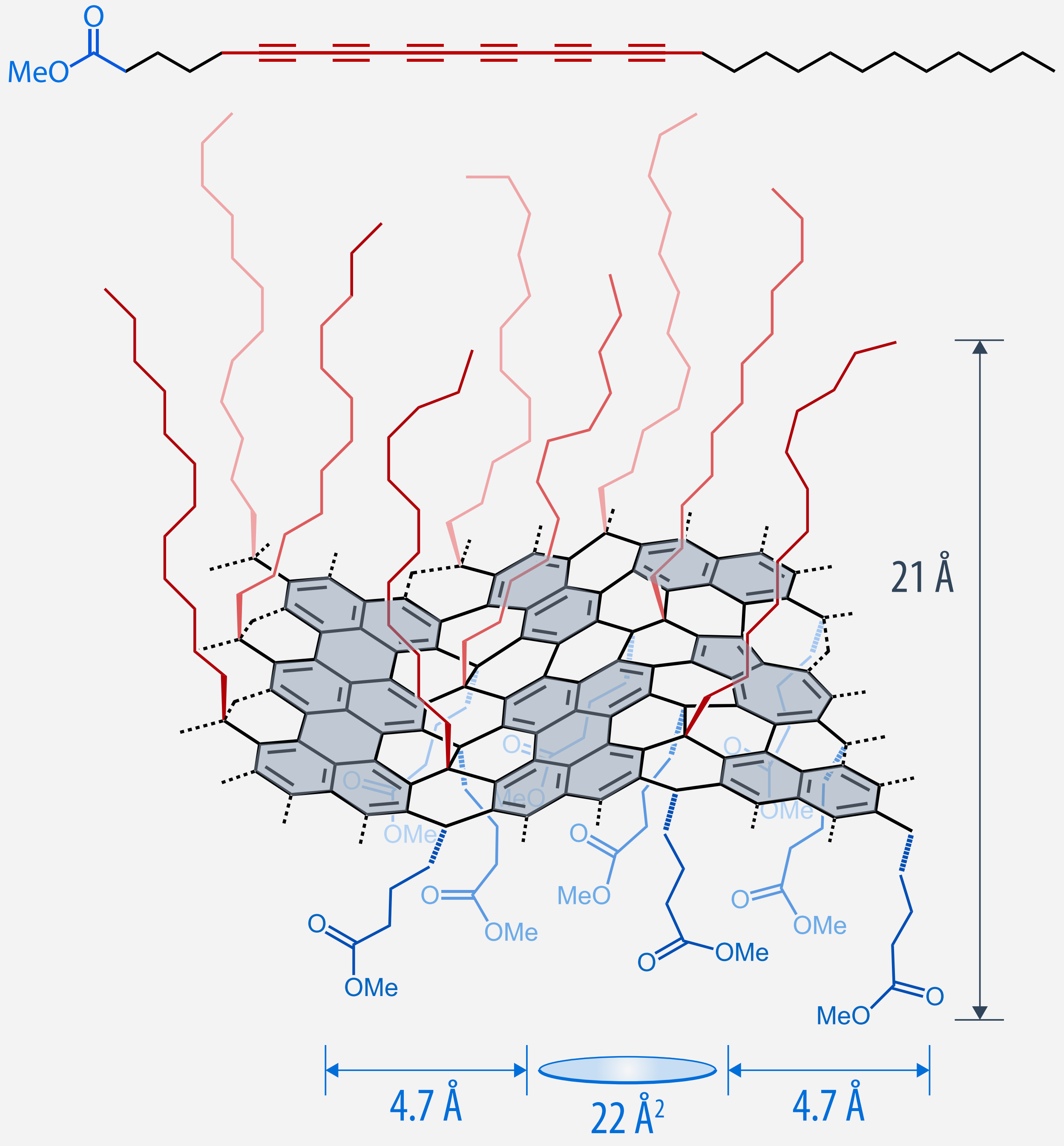
organic semiconductor
nanostructures

mechanical properties



hierarchically structured
supramolecular materials

chemical reactivity



carbon nanomaterials
at room temperature

- **control of the balance of order and disorder across length scales to tailor structure and function**

From Molecular Design to Materials and Devices

molecular design & synthesis

synthetic chemistry,
NMR, MS, MALDI

physicochemical characterization

UV/vis/NIR, CD, fluorescence,
IR, Raman, ESR, DLS, CV

materials processing

extrusion, drawing, blowing,
injection molding, microfluidics

materials characterization

AFM, TEM, SEM, SAXS, WAXD
rheology, DMA, mechanical testing

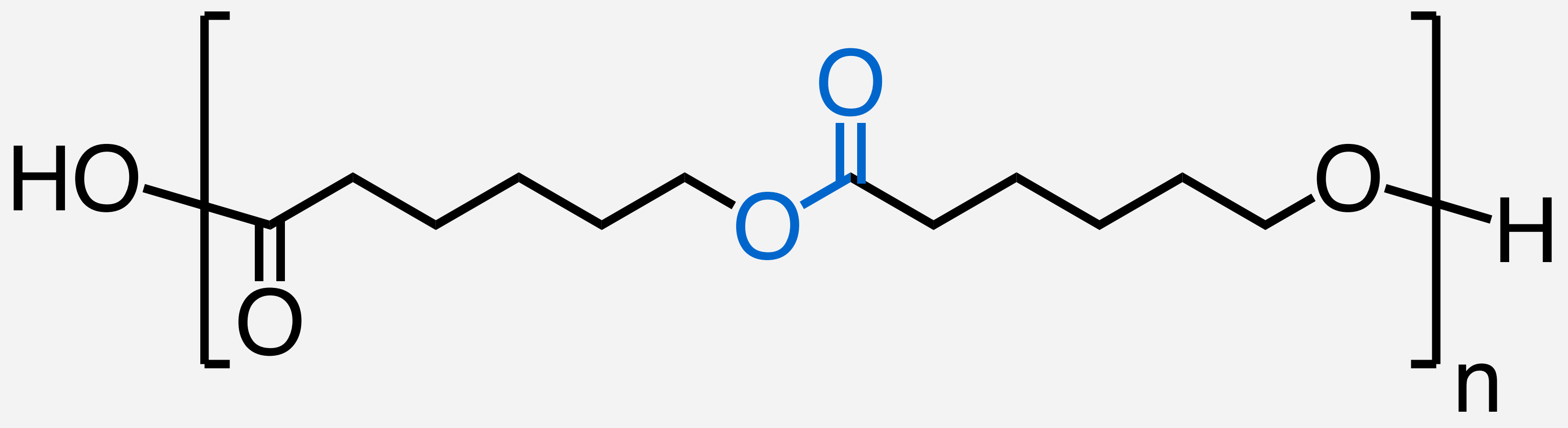
device fabrication

damping structures, railpads,
food containers, OFETs

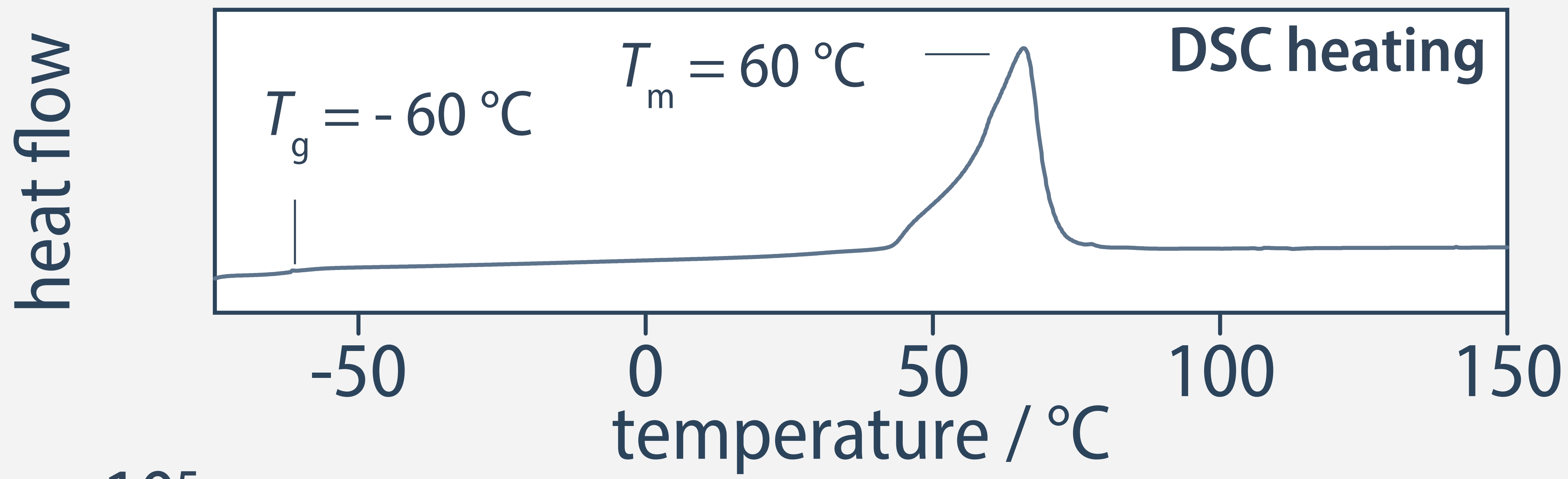
device testing & applications

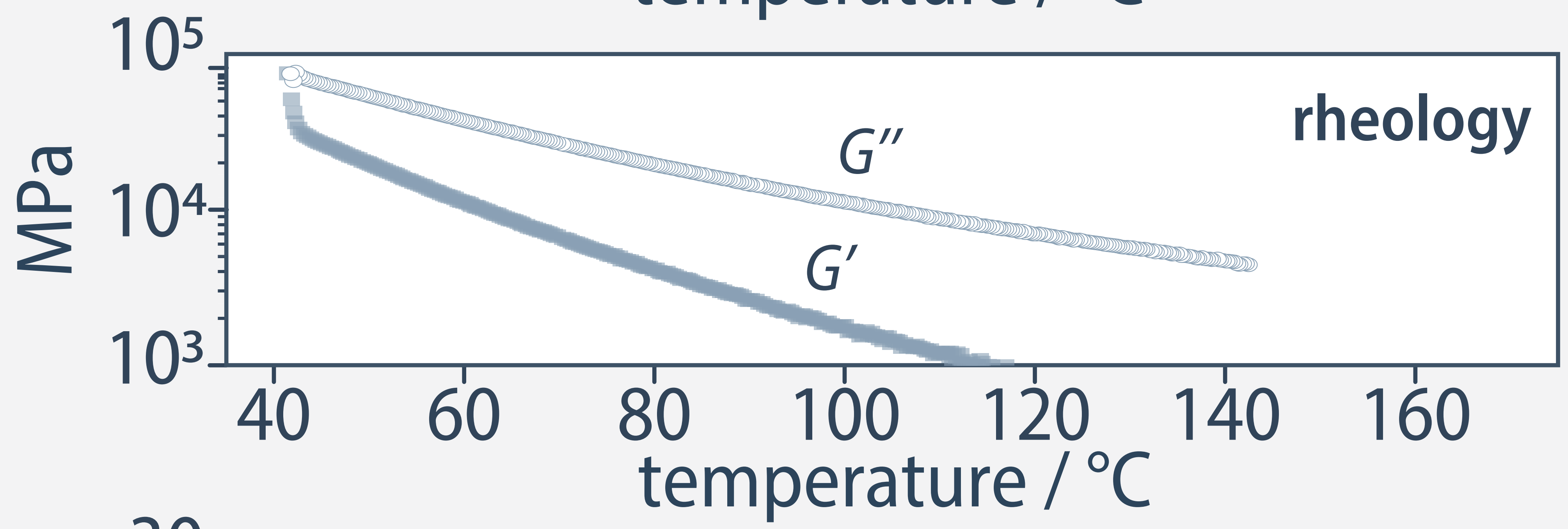
damping, acoustics, barriers,
packaging, recycling, degradation

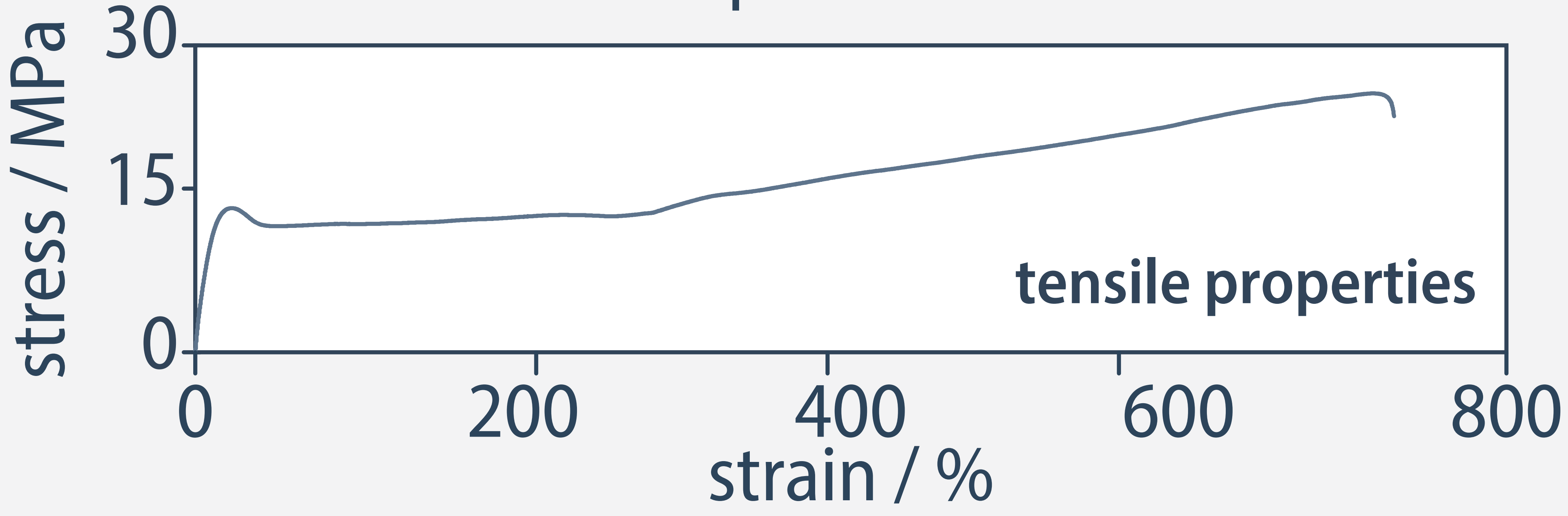
Poly(ε-caprolactone) (PCL) - A Biodegradable Aliphatic Polyester



- polyethylene-like properties
- petroleum-based or bio-based
- hydrolytically cleavable ester groups
- FDA-approved
- implantable biomaterial
- biodegradable



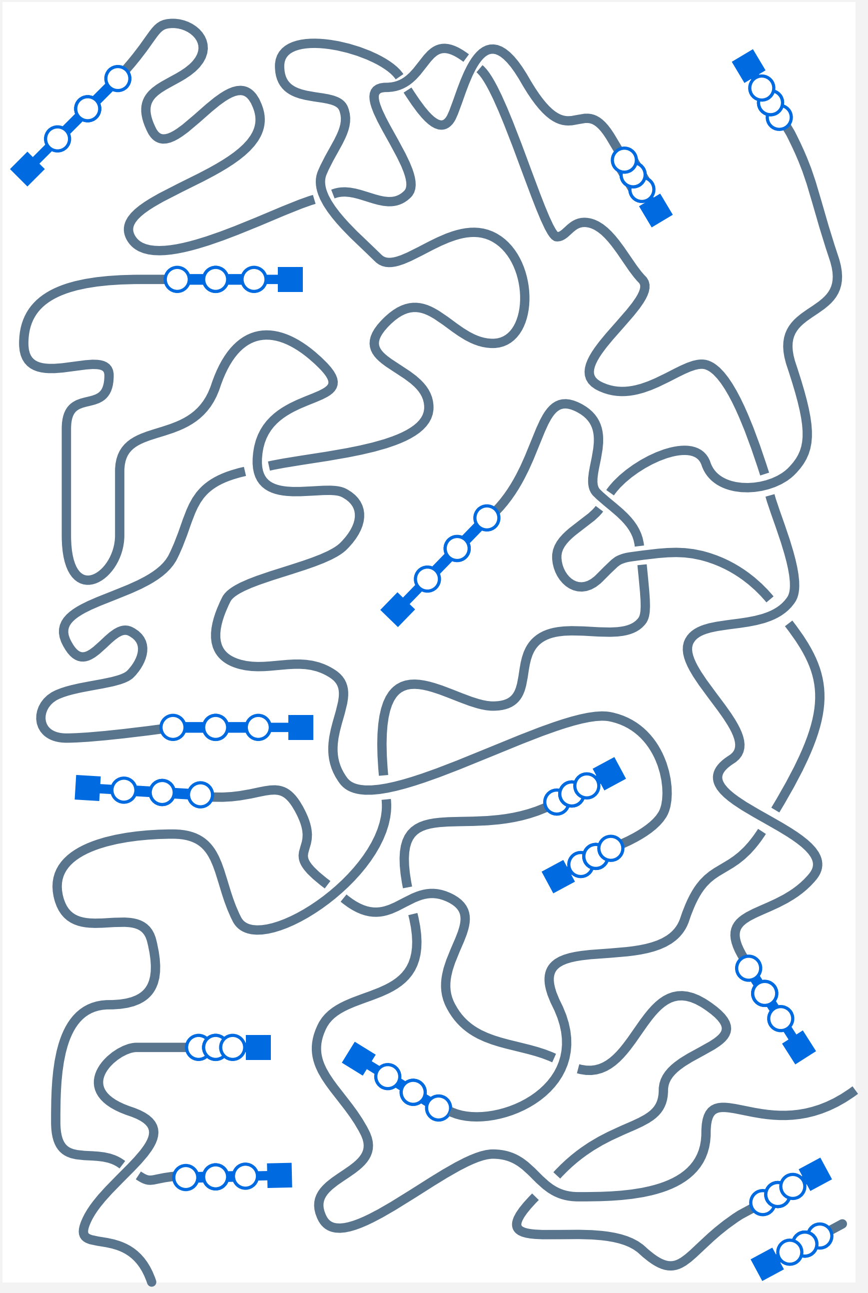




- **PCL has limited engineering applications due to poor thermal, rheological & mechanical properties**

End Group and Additive Co-Assembly

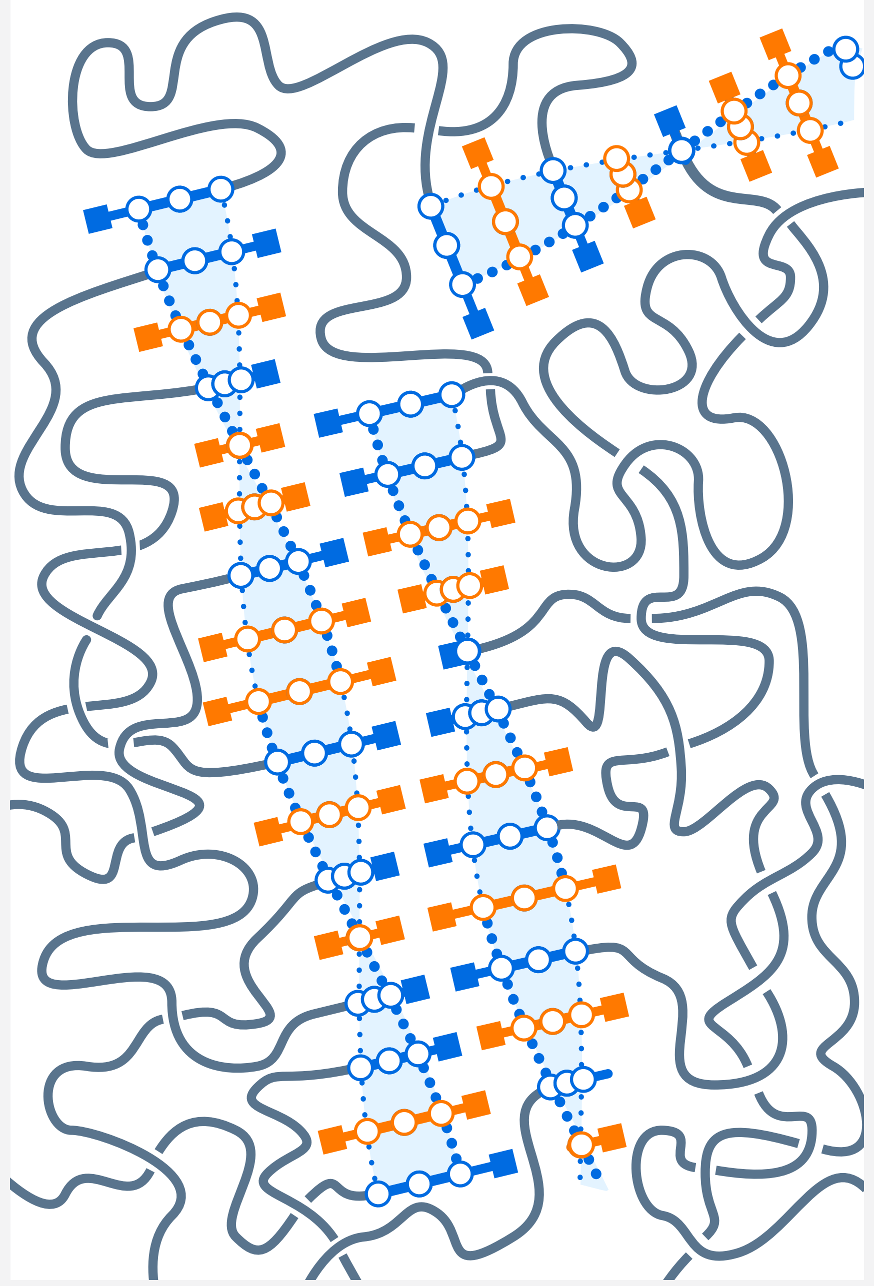
- problem: high polymer molecular weight and end group aggregation are mutually exclusive
- solution: reinforcement by co-assembly of ditopic polymer end groups and a matching additive



without additive:
poor network formation

high molecular weight polymer with
ditopic hydrogen-bonded end groups

reinforcing additive using the
same supramolecular motif

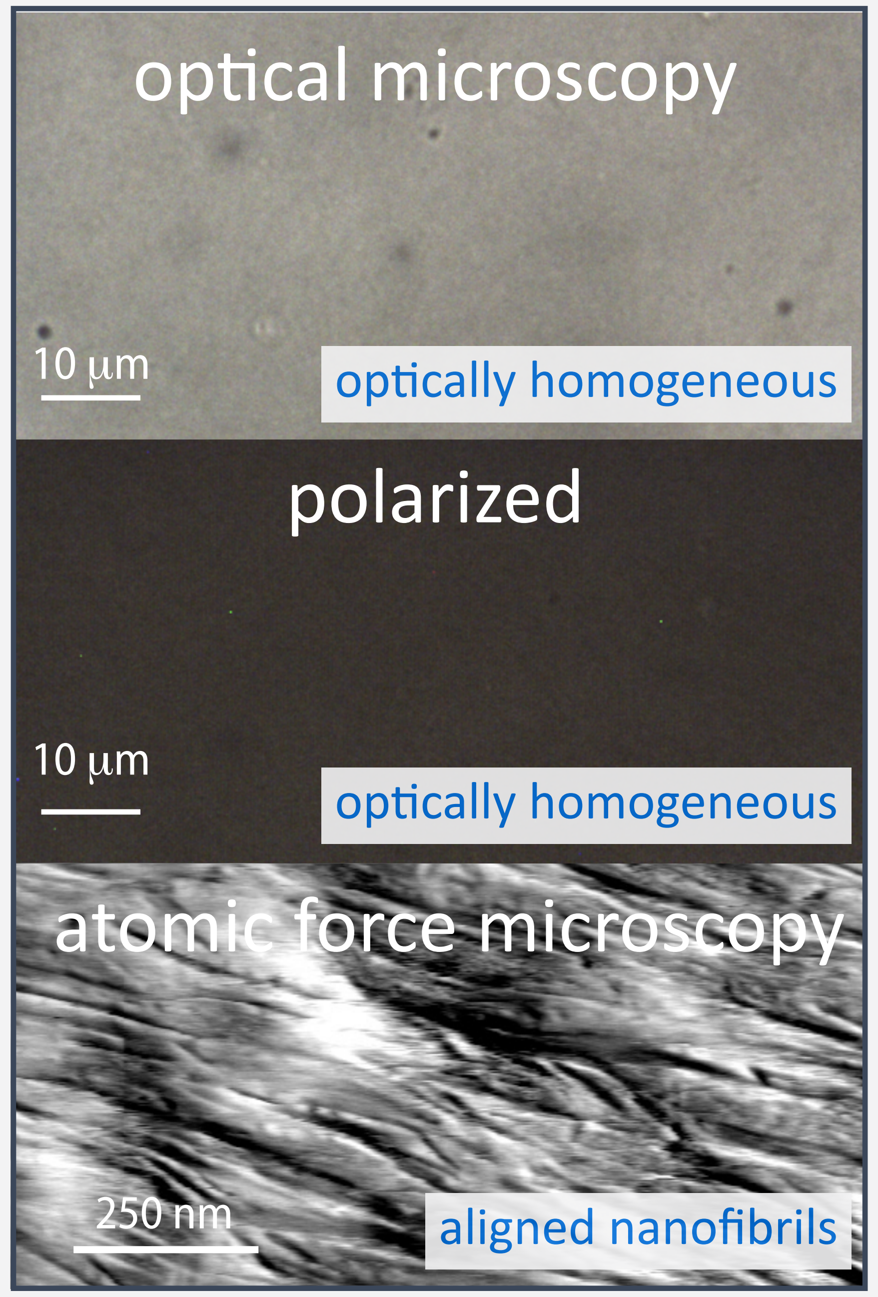


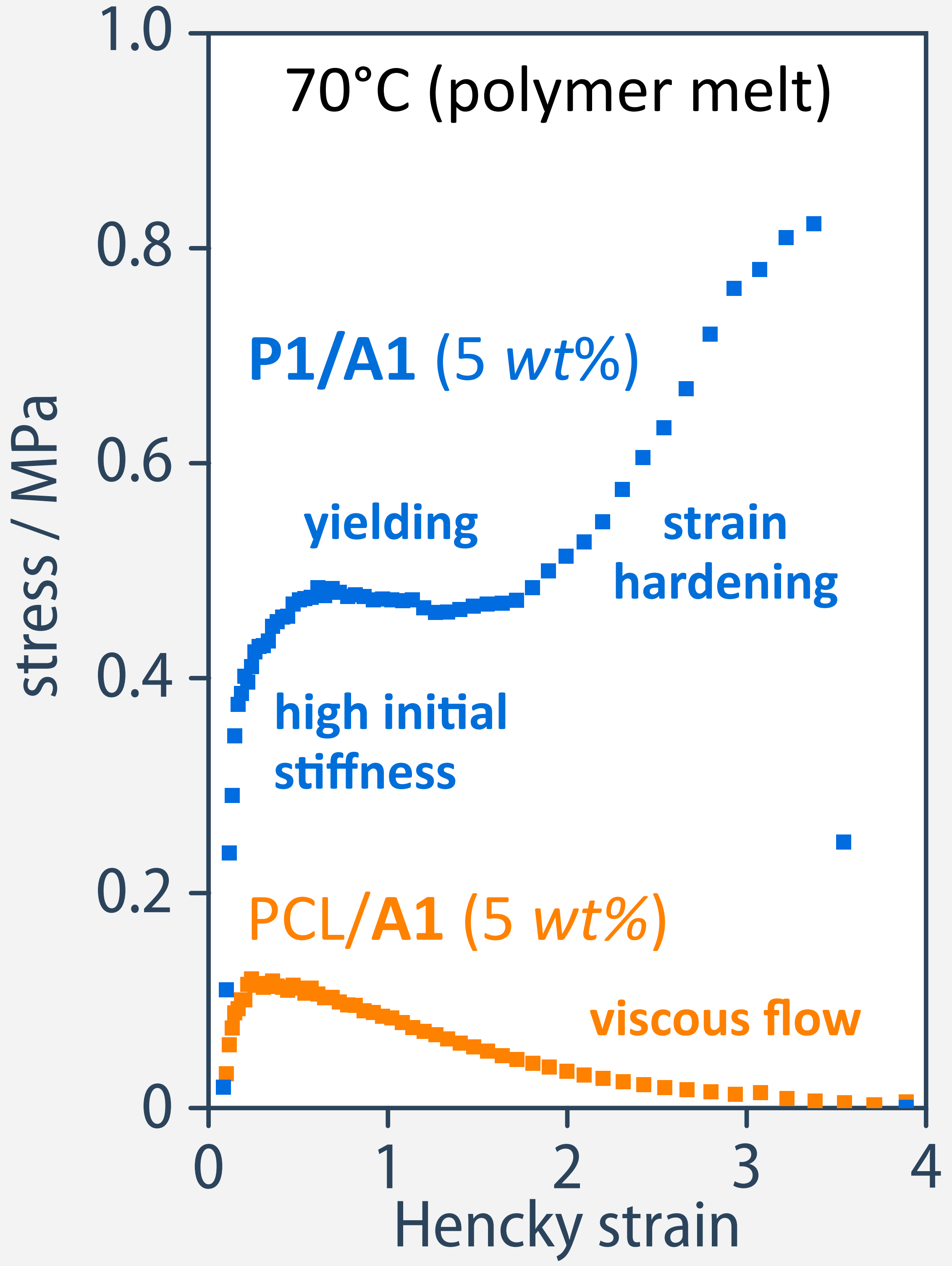
co-assembly into reinforced
nanofibril aggregates

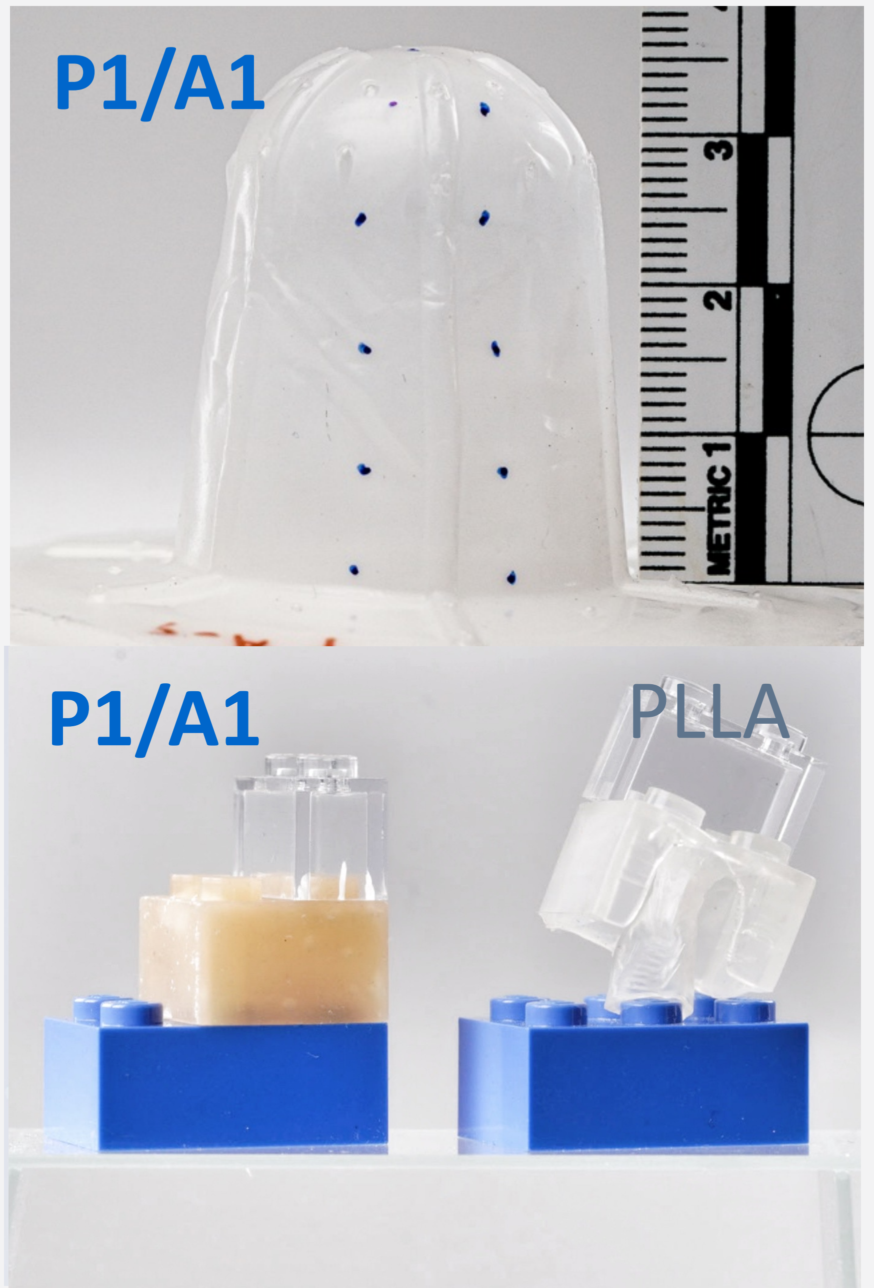
- **tailorable property profiles based on supramolecular networks independent of molecular weight**

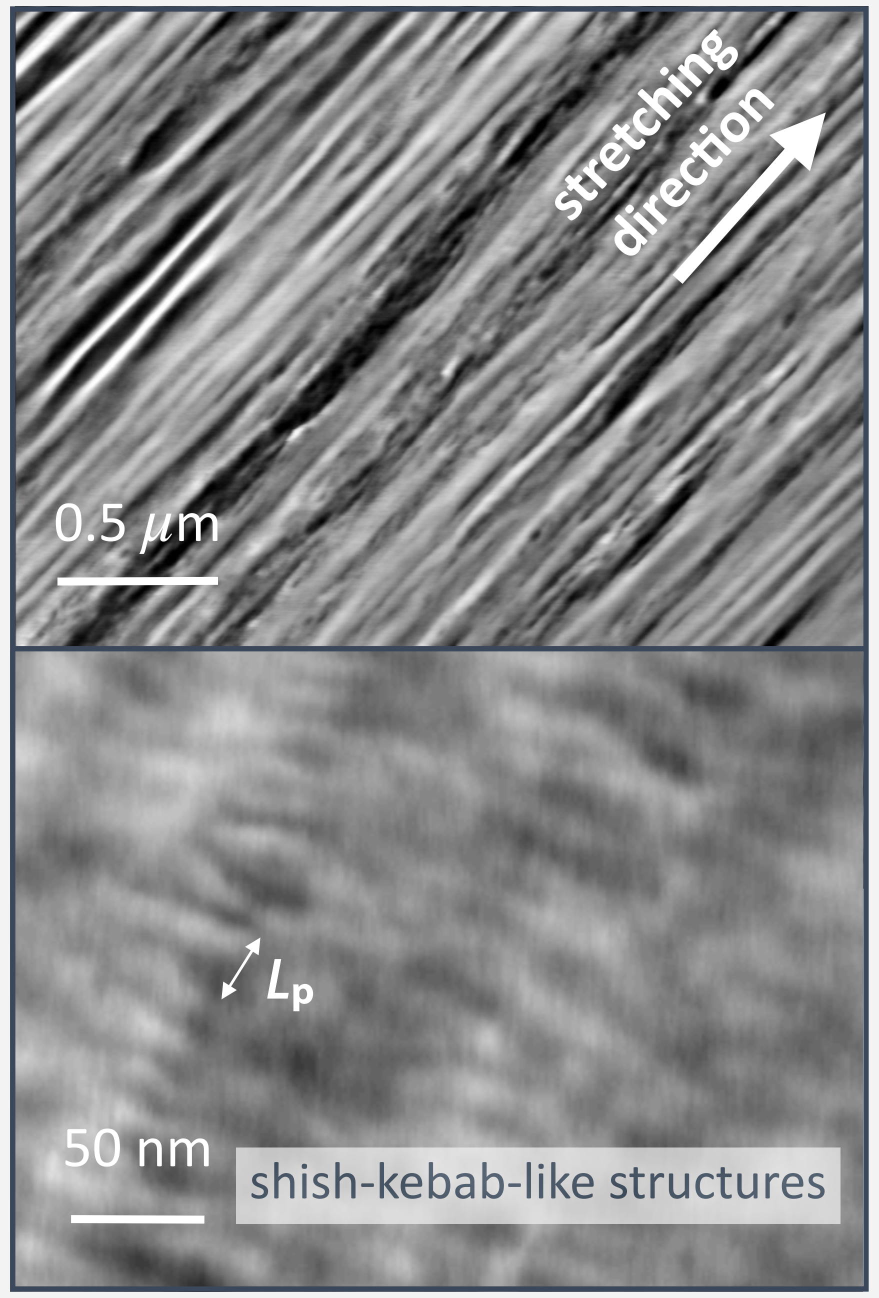
Supramolecular Modification for Tailored Melt Properties and Product Performance

new nanofibril phase regime ▶ **tailored melt strength & elasticity** ▶ **new / improved processing options** ▶ **materials orientation**









cross-linking reinforcement ▶ **melt deformation strain hardening** ▶ **processing at high deformation** ▶ **high draw ratios fibrillar crystals**

Learning Outcomes

- organic chemistry is the basis for polymer science and soft matter research
- soft matter research has increased in relevance in our department
- relevance will further increase with focus on sustainable materials