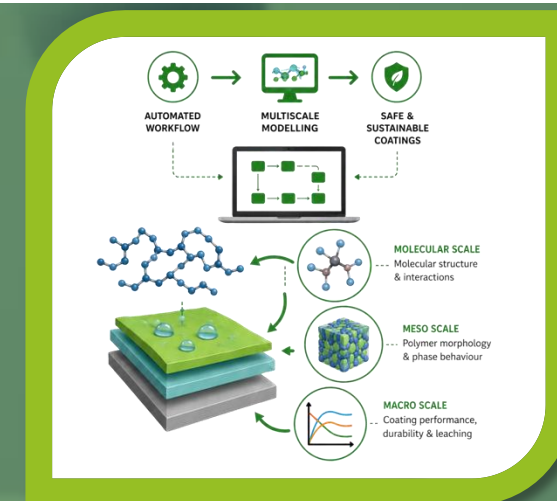




3rd Training

INTRODUCTION TO AUTOMATED MULTISCALE PHYSICS-BASED MODELLING FOR SAFE & SUSTAINABLE COATINGS

June 16, 2026
Online



Agenda

10:00 Opening Remarks and Introduction

- Goal of the training and overview
- BIO-SUSHY brief project intro (5-10 min)



10:15 Module 1 - Multiscale Modelling

- Importance of physics-based modelling for SSbD (20 min)



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Introduction

PFAS, What?

PFAS (per and polyfluorinated alkyl substances) provide excellent **water** and **oil repellency** properties.

Why is it a problem?

PFAS are known as '**forever chemicals**' due to their resistance, widespread, and linked to **environmental** and **health problems** like cancer and decreased fertility.

How?

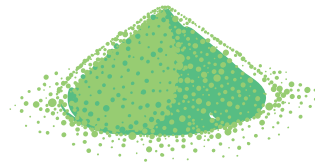
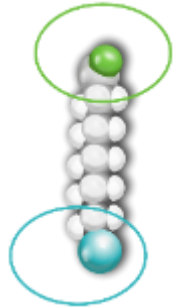
Exposure could happen through **eating**, **drinking**, or **using** consumer products containing PFAS.

You may have assumed PFAS without knowing it



Objectives

Develop **3 PFAS-free bio-based coatings**



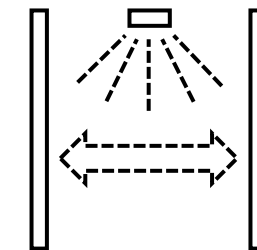
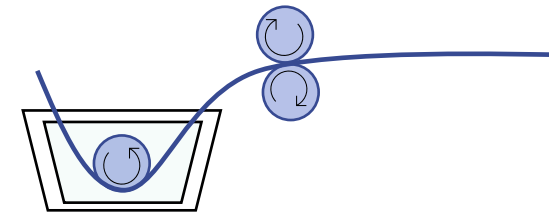
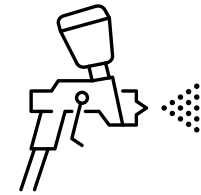
Thermoplastic bio-based **powder**



Water-based **hybrid sol-gel** organic



Solvent-based **hybrid sol-gel** inorganic



Hydro/oleophobic
additives



R&I Coating Development



TEXTILE COATING



FOOD PACKAGING



GLASS COSMETICS
PACKAGING

- Development of **3 novel SSbD coatings materials** with water and oil repellency
- **Validation** of coating materials with 3 case studies
 - Textile
 - Food packaging
 - Glass packaging

BIO-SUSHY Methodology – Based on 3 pillars



R&I COATING DEVELOPMENT

- Development of 3 novel SSbD coatings materials with water and oil repellency
- Validation of coating materials with 3 case studies (cellulose food trays, textile, glass packaging)



MODELING

- Development of the BIO-SUSHY set of computation tools for SSbD of coatings
- Development of integrated approaches supported by the BIO-SUSHY HUB for effective data management and sharing



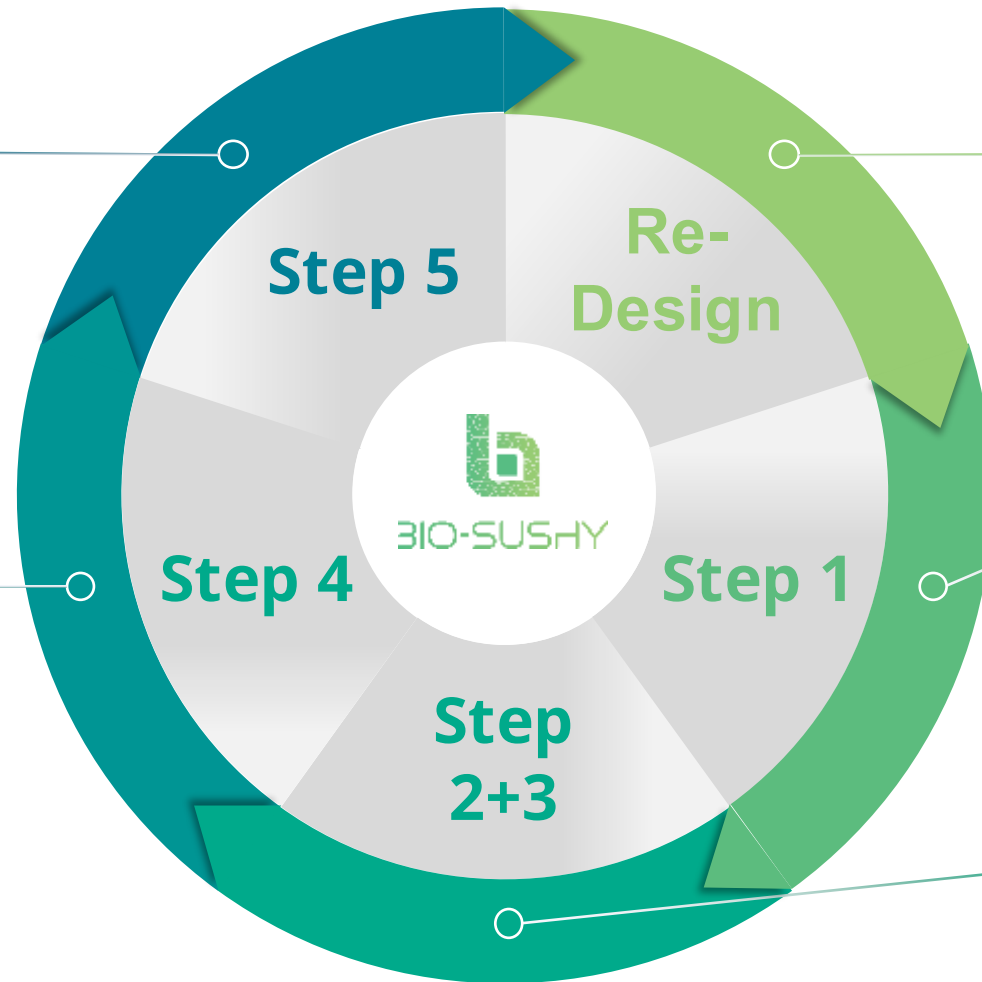
SAFE AND SUSTAINABLE BY DESIGN

- Development of an SSbD Framework applied to PFAs-free coatings (safe by material design, safe by process design, toxicological studies, LCA, LCC, SLCA)
- Standardisation roadmap



The 5 steps SSbD framework

- Life Cycle Costing (LCC)
- Social-LCA
- LCA
- Circularity
- End of life



- Coating development
- Functional modelling
- Data mining
- Up-scaling

- Data mining
- QSAR

- Occupational monitoring
- Risk assessment
- Tox testing

Unique value proposition

Coatings validated in 3 case studies

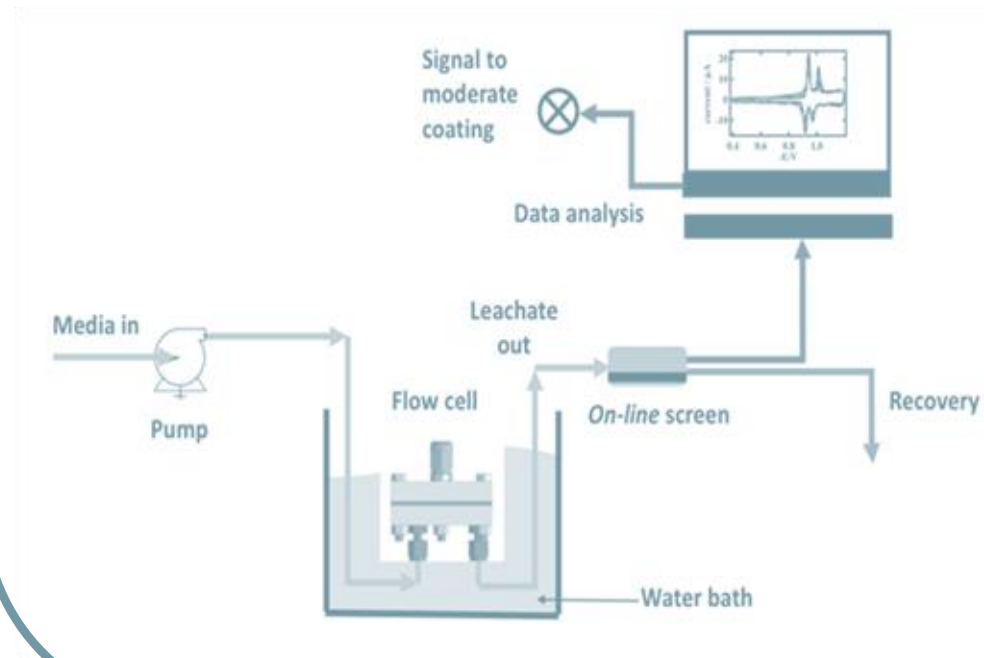


Textile

Food trays and packaging

Glass cosmetic packaging

Rapid coating and formulation screening



Standardisation & SSbD framework

- Standardisation of new coatings
- Definition of safety and sustainability criteria

Impacts



**25% reduction of
environmental
impact**



**Contribution to
SSbD criteria and
guiding principles**



**Reduction of PFAS
in the
environment**



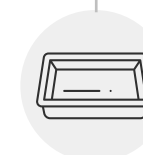
**Computational
tools to support
SSbD concepts**

Value Chain

BIO-SUSHY consortium combines **materials science, sustainability assessment, and industrial validation**



Applications

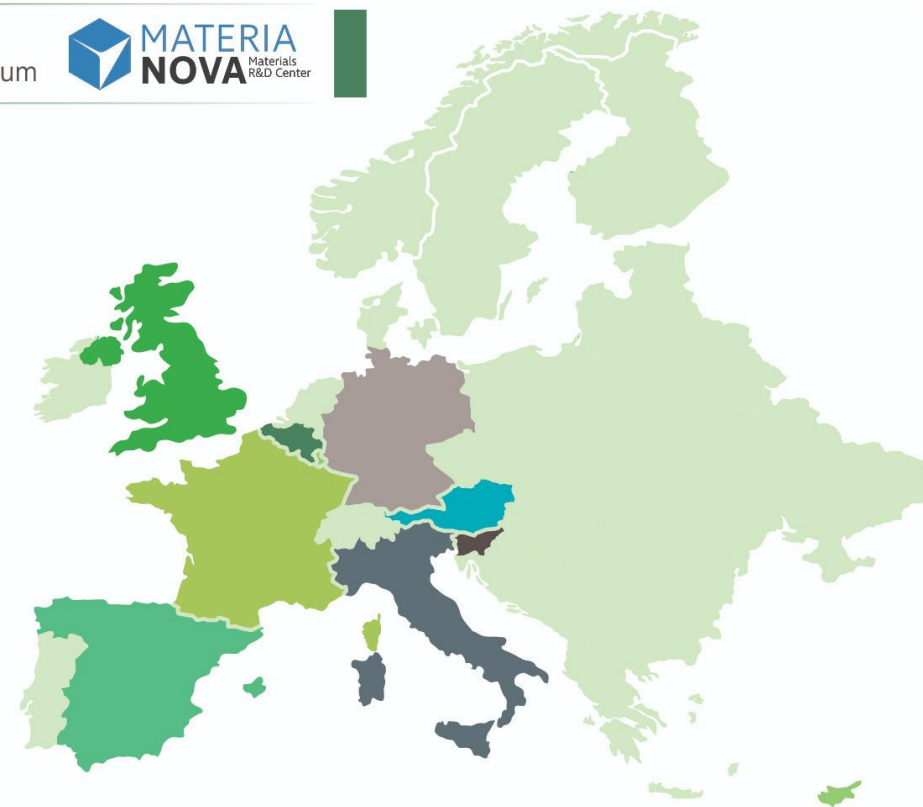


Team

The **BIO-SUSHY** project is a collaboration between 14 partners from 7 EU countries and 1 EU-associated country: 6 RTDs, 6 SMEs, 1 university, and 1 national association.

BIO-SUSHY COORDINATOR:

Materia Nova, Av. Nicolas Copernic 3, 7000 Mons, Belgium



BIO-SUSHY SSbD Guidelines



SSbD Guidelines - Food Packaging



SSbD Guidelines - Glass Cosmetic Packaging



SSbD Guidelines - Textile



SSbD Guidelines Infographic - Food Packaging



SSbD Guidelines Infographic - Glass Cosmetic Packaging



SSbD Guidelines Infographic - Textile

<https://www.bio-sushy.eu/dc-materials/>



 **WORKSHOP**

13 OCTOBER 2026

 Hotel Van der Valk
 Avenue M.Mercuri Mons (B)

HOW COATINGS
SUPPORT CIRCULARITY OF
MATERIALS

[Program](#)

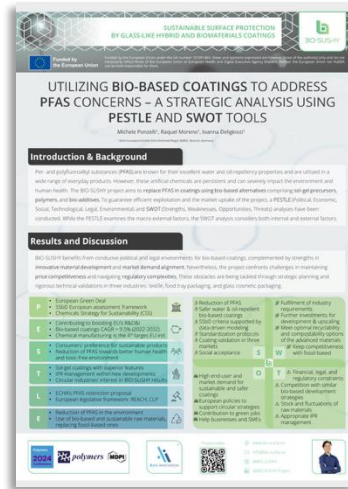
[Registration](#)

Stay up to date with our progress



www.bio-sushy.eu

info@bio-sushy.eu



@BIO-SUSHY Project



@BIO_SUSHY

Dr. Andrea Lorenzoni

Researcher

Consiglio Nazionale delle Ricerche (CNR)



Dr. Francesco Mercuri

Senior Researcher

Consiglio Nazionale delle Ricerche (CNR)



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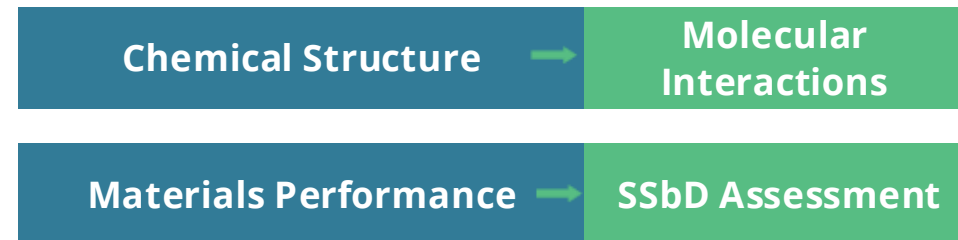
WHY MODELLING MATTERS FOR SSbD COATINGS

Development of PFAS-free and bio-based coatings requires understanding material behaviour before large-scale experimental testing.

Modelling enables:

- Faster screening of candidate materials
- Reduction of costly trial-and-error experiments
- Prediction of performance before synthesis
- Understanding molecular mechanisms driving functionality
- Assessment of leaching and migration risks
- Support for SSbD decisions

Modelling workflow:




KEY MESSAGE

*Experiments tell us what happens. Modelling helps explain **why** it happens and predict **what may happen next**.*

FROM CHEMISTRY TO PERFORMANCE: A MULTI-SCALE PERSPECTIVE

Scale	Typical Methods	Information Obtained
Molecular	Molecular Dynamics, Quantum Chemistry	Molecular structure, interactions, diffusion mechanisms
Mesoscale	Coarse-Grained Models	Morphology, aggregation, phase behaviour
Bulk Materials	MD Simulations, Continuum Models	Density, mechanical response, transport properties
Surfaces	Interface Simulations	Surface energy, adsorption, wettability
Framework	Multi-scale Workflows	Leaching potential, performance indicators, SSbD metrics

Multi-scale information flow: Chemistry → Structure → Morphology → Properties → Performance → Sustainability

 **KEY MESSAGE** | *Material performance emerges from phenomena occurring across **multiple length and time scales**.*

THE BIO-SUSHY PHYSICS-BASED MODELLING PHILOSOPHY

Modular, multiscale and automated

BIO-SUSHY adopts a workflow-oriented modelling strategy designed to support material development and assessment.



Modularity

- ◆ Independent simulation components
- ◆ Reusable workflows
- ◆ Flexible integration of new materials and use cases
- ◆ Flexible integration of new materials and use cases

Automation & Integration

- ◆ Standardised protocols
- ◆ Reproducible simulations
- ◆ Automated generation of materials descriptors and data → AI models
- ◆ Automated integration in the BIO-SUSHY registry




Physics-Based

- ◆ Mechanistic understanding, not black-box predictions
- ◆ Explicit connection between chemistry and material behaviour
- ◆ Interpretable outputs supporting SSbD assessment

Workflow structure:



 **OBJECTIVE** | *Not only to predict properties, but to understand the **physical mechanisms** linking materials properties to performance and sustainability.*

Automated workflows developed within BIO-SUSHY



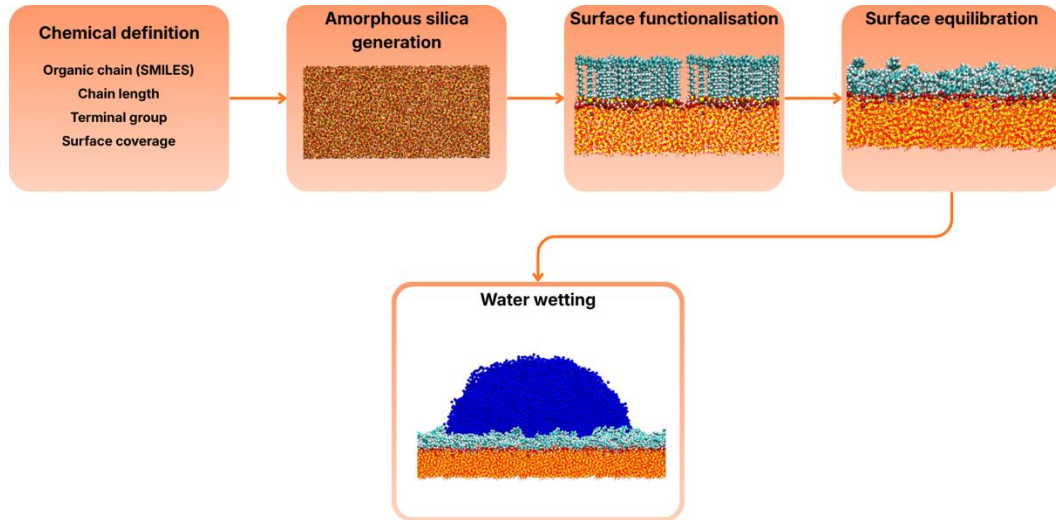
- Development of **3 novel SSbD coatings materials** with water and oil repellency

Terminal Function
Tailored to the targeted properties / applications

Grafting Function
Adjusted to the chemical nature of the materials to modify

- **Validation** of coating materials with 3 case studies
 - Textile
 - Food packaging
 - Glass packaging

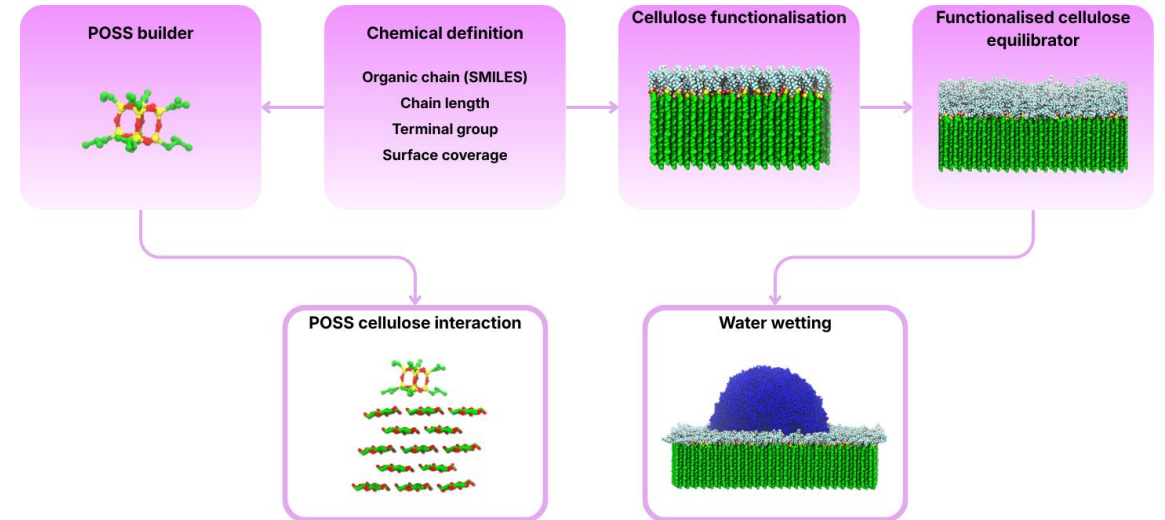
Glass packaging workflow



Experimental demonstrator



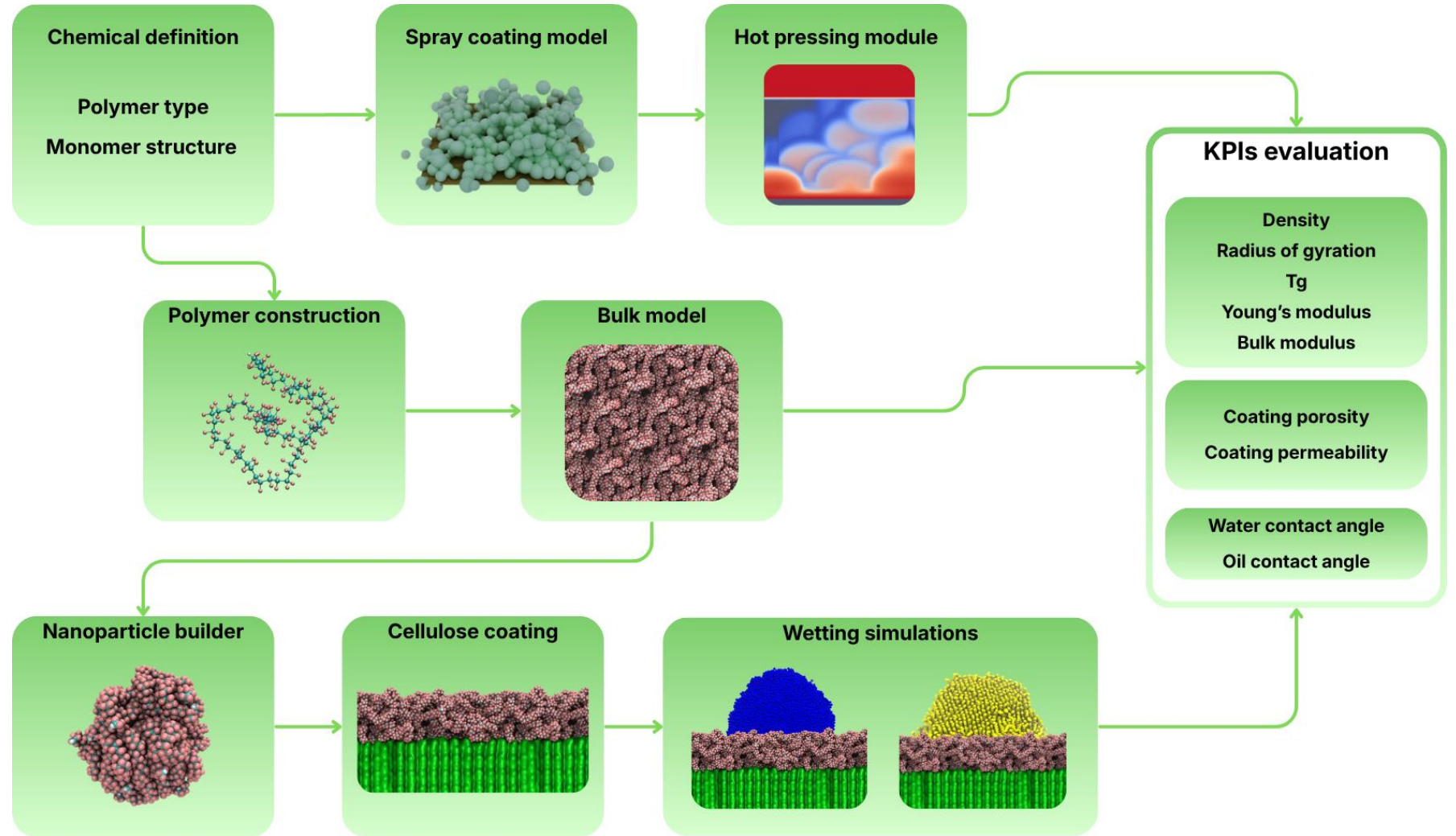
Textile workflow



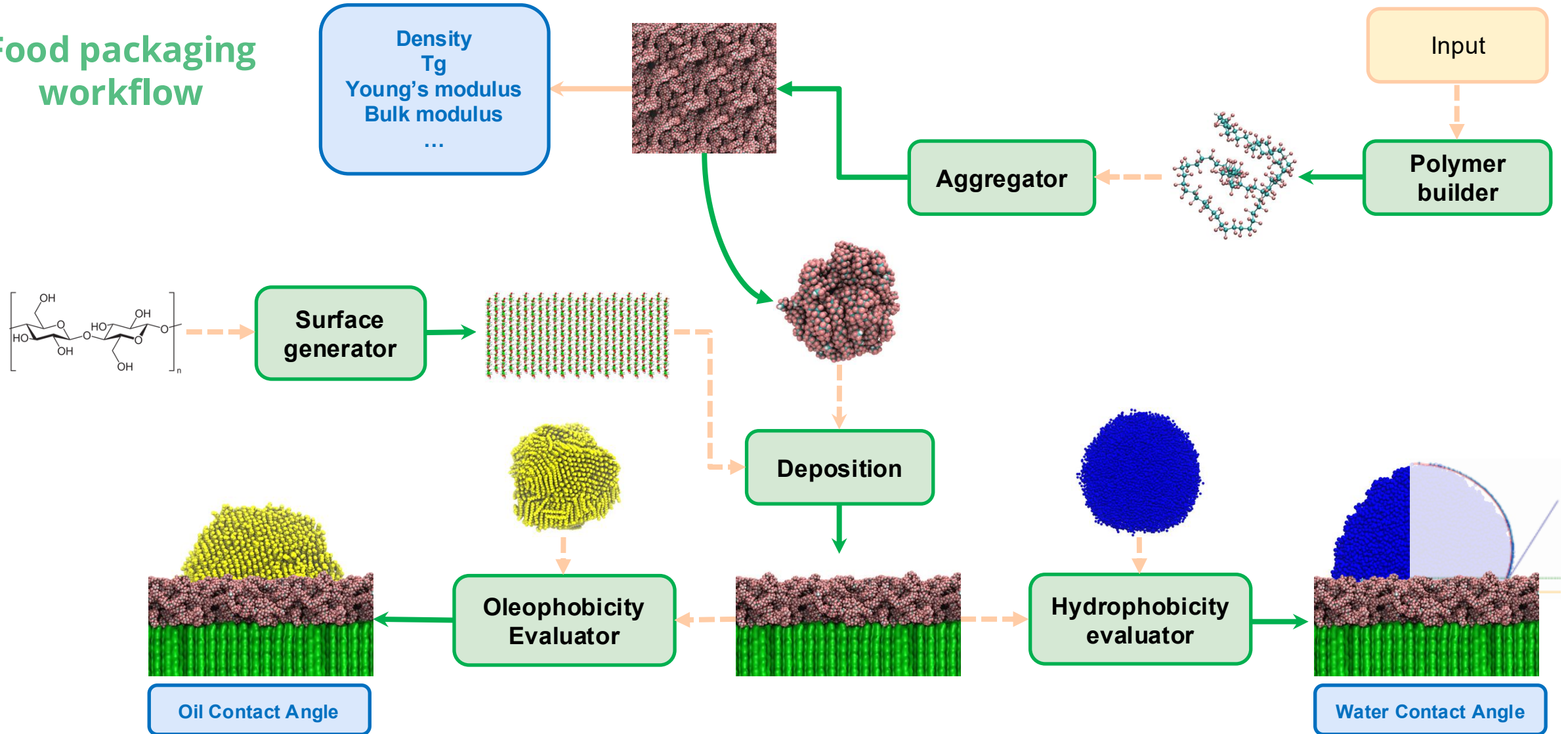
Experimental demonstrator



Food packaging workflow



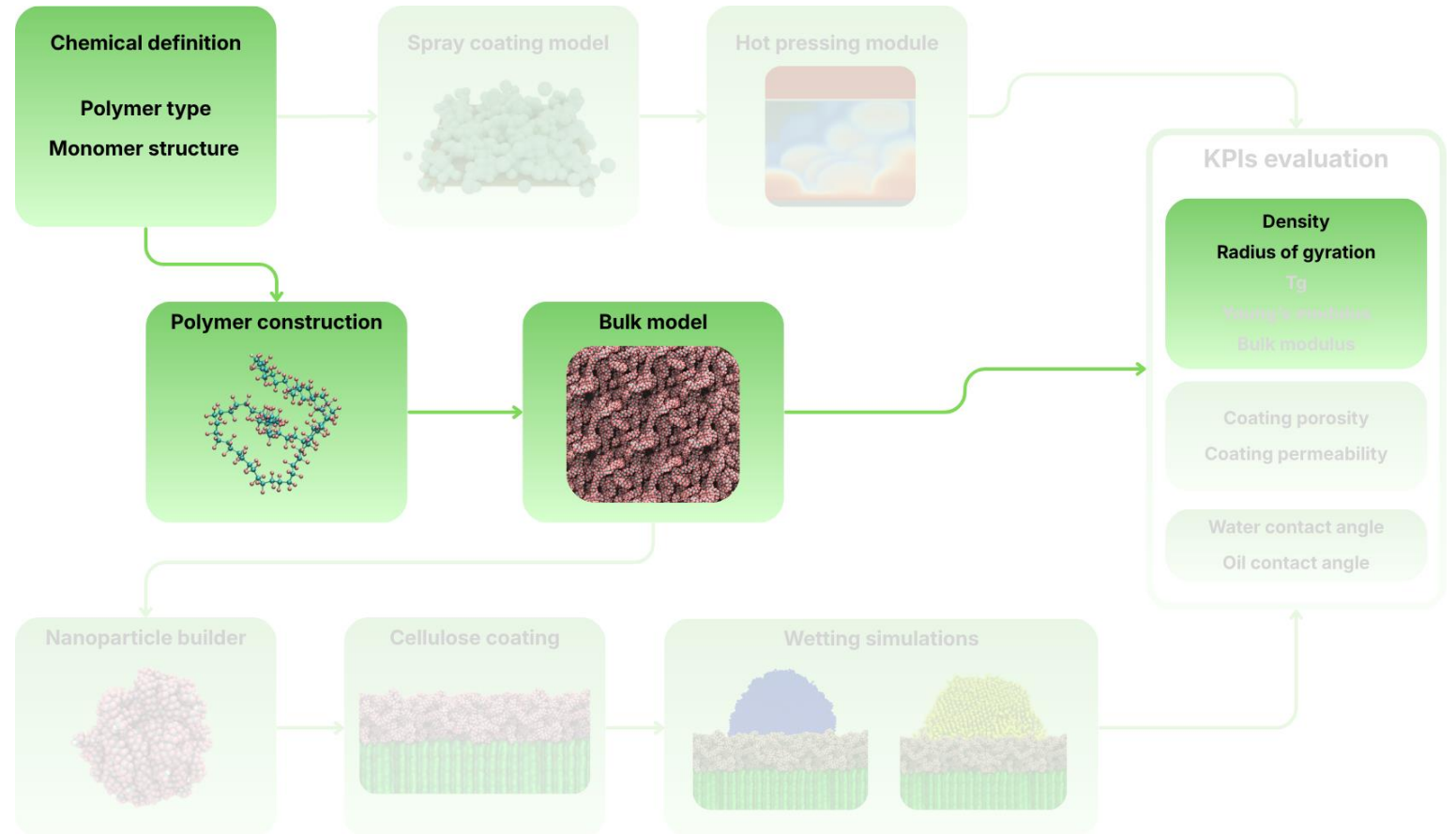
Food packaging workflow



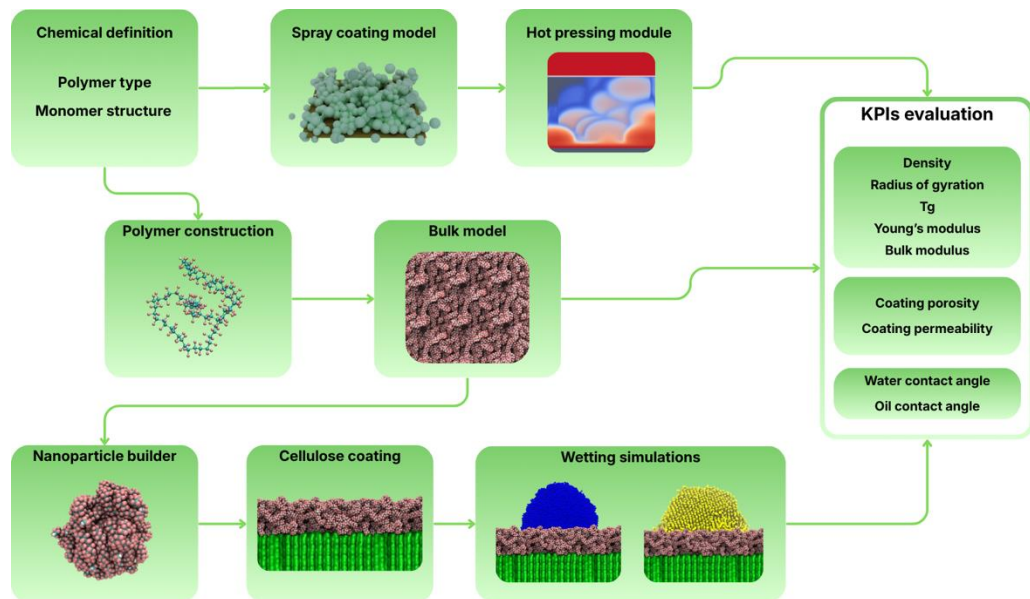
Module 2: Hands-on Simulations

[Link to the Tutorial](#)

- ❖ Generation of polymer chains from simple chemical inputs
- ❖ Force-field parametrisation
- ❖ Short MD simulations
- ❖ Bulk system generation
- ❖ Extraction of simple materials descriptors



Food packaging workflow - Results



Polymer	Density (g/cm ³)		Young's modulus (Gpa)		WCA (°)	
	Sim	Exp	Sim	Exp	Sim	Exp
PS	1.02	1.05 - 1.07 ¹	2.4	1.9 - 2.9 ¹	93	86 ⁵
PMMA	1.11	1.18 - 1.19 ¹	3.0	2.4 - 3.4 ³	73	68 ⁶
PTFE	1.98	2.1 - 2.2 ¹	0.46	0.4 - 0.8 ⁴	119	116 ⁷
PHBV	1.13	1.25 ²	1.7	2.4 - 3.6 ²	82	79 ⁸

¹ <https://matmake.com/properties/youngs-modulus-of-polymers-and-plastics.html>

² <https://doi.org/10.3390/polym12061300>

³ https://www.engineeringtoolbox.com/young-modulus-d_417.html

⁴ <https://doi.org/10.1016/j.polymer.2004.08.064>

⁵ <https://doi.org/10.1021/la0636311>

⁶ <https://doi.org/10.1016/j.polymer.2007.10.038>

⁷ <https://doi.org/10.1002/mame.202200617>

⁸ Data from experimental partners of BIO-SUSHY (WOOD-KPLUS)

Take-home messages

- ❖ Molecular simulations provide SSbD-relevant descriptors linking structure, real-life process and material properties
- ❖ Automation and modularity enable reproducible, high-throughput and scalable material screening
- ❖ Integration with AI frameworks can accelerate the identification of safer and more sustainable material candidates

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WEB: www.bio-sushy.eu

EMAIL: info@bio-sushy.eu

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Horizon's Europe GA number: 101091464