
TNO innovation for life
AI to design new packaging materials
polySCOUT
POLYMER DESIGN
BY MACHINE LEARNING

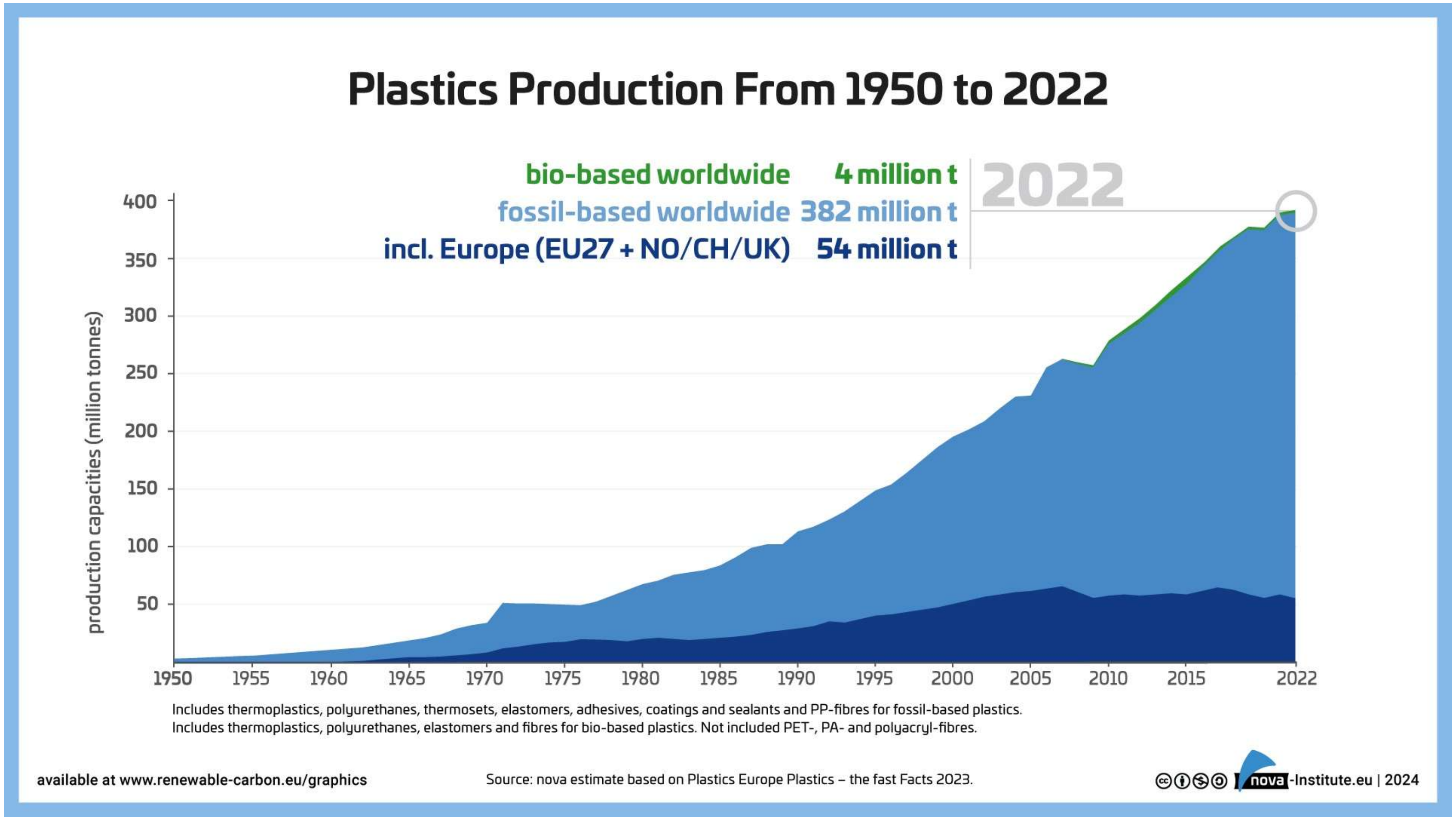
Plastics:
the good, the bad & the ugly

- Useful and omnipresent
- Cheap
- Tuneable properties
- Durable &Lightweight
- Sustainability transition

- Development time & cost
- Dependence on experts
- Fossil feedstocks
- End-of-Life, Microplastics
- Unsafe chemistries (toxic)

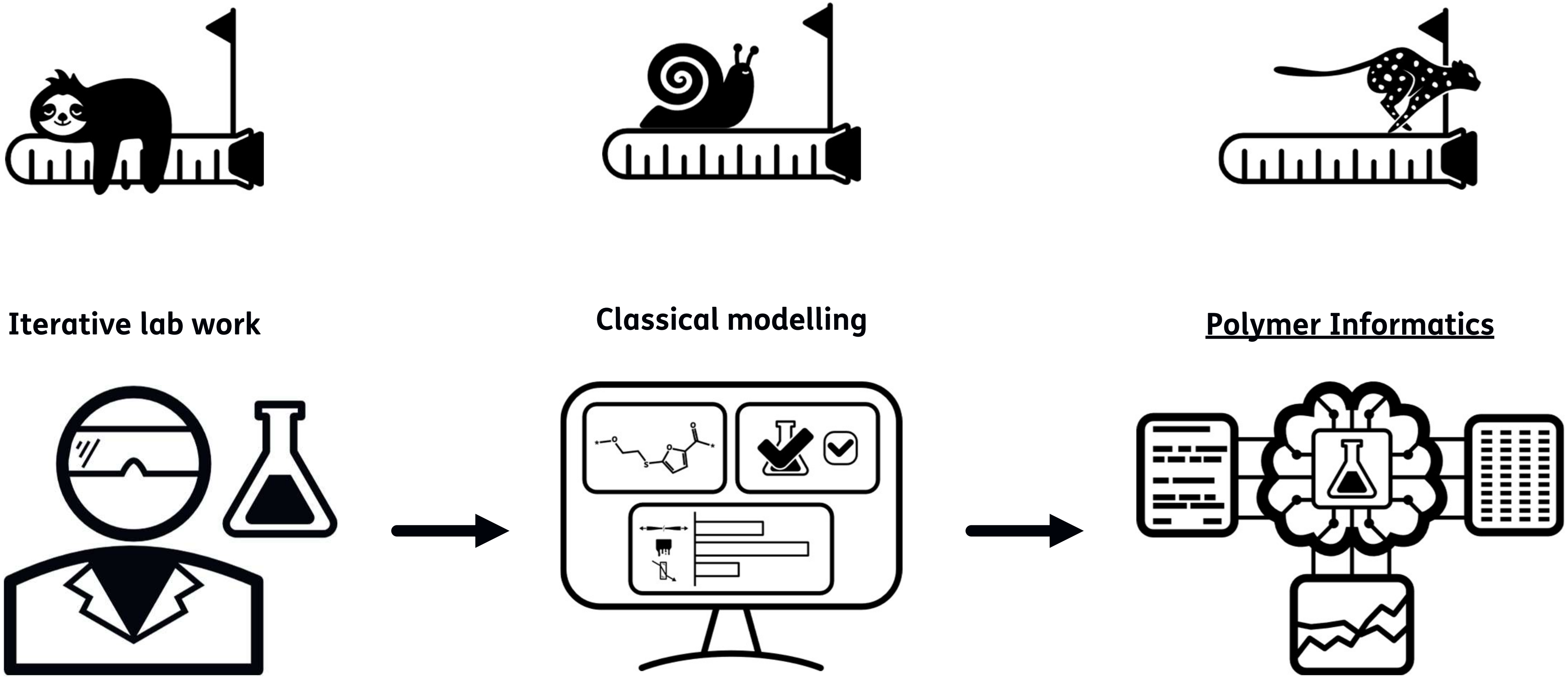
We need (novel) safe & sustainable materials.

… and we need to accelerate! But how?



ENTER AI.

Impact of AI: acceleration of R&D



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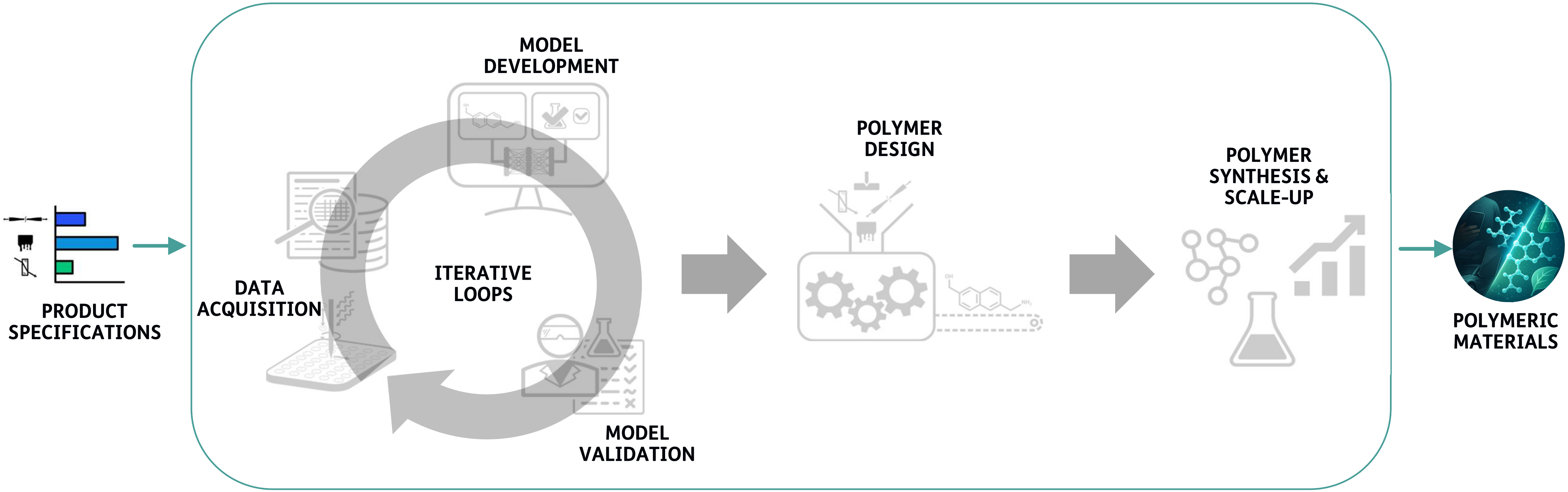
polySCOUT: blending AI, polymer science and testing for material design & development



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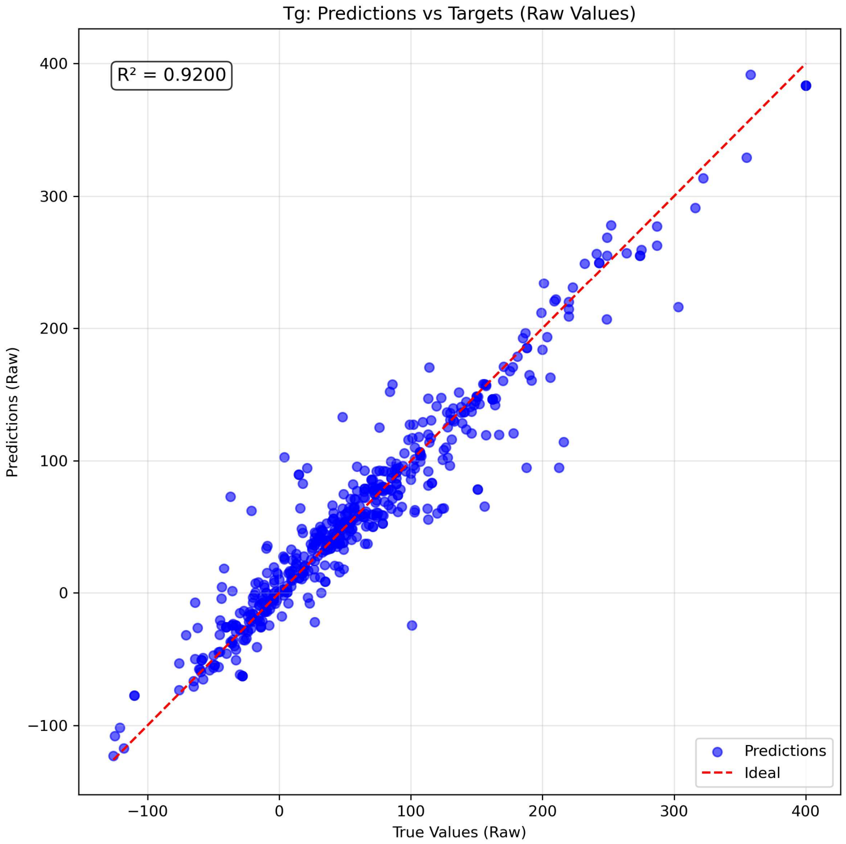
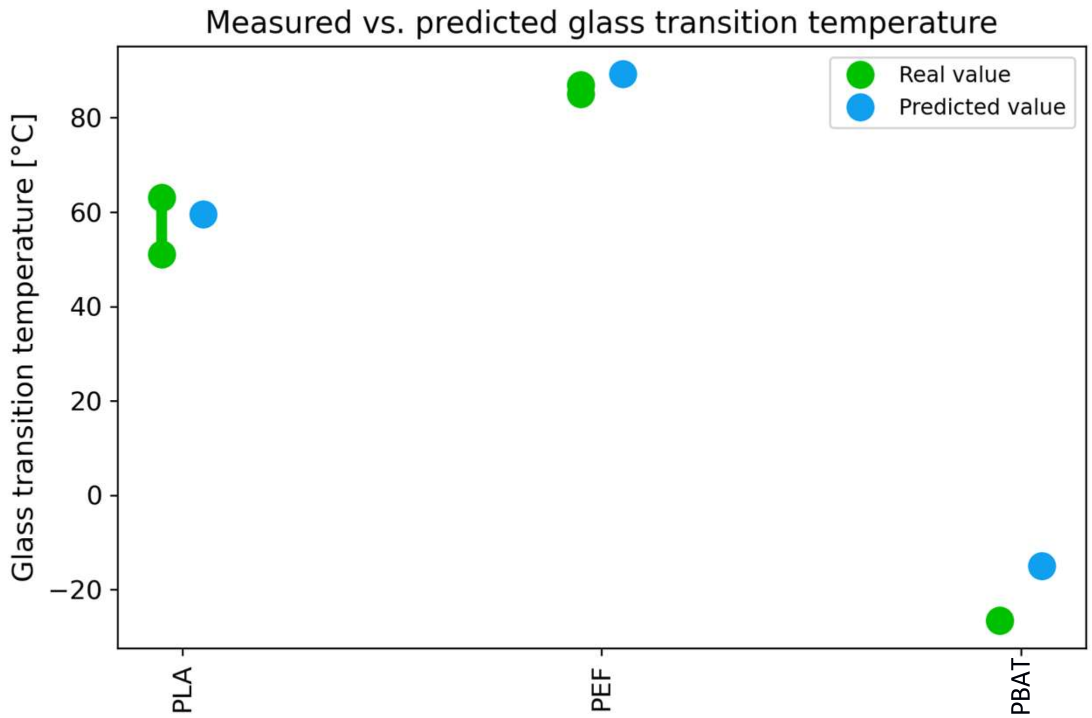
Well-performing model!

We built our own high-quality curated dataset
~5000 polymers (>90% polycondensates)
~9000 datapoints
We trained our own AI-models



Overall performance of model for Tg



Comparison for 3 known (biobased) polymers

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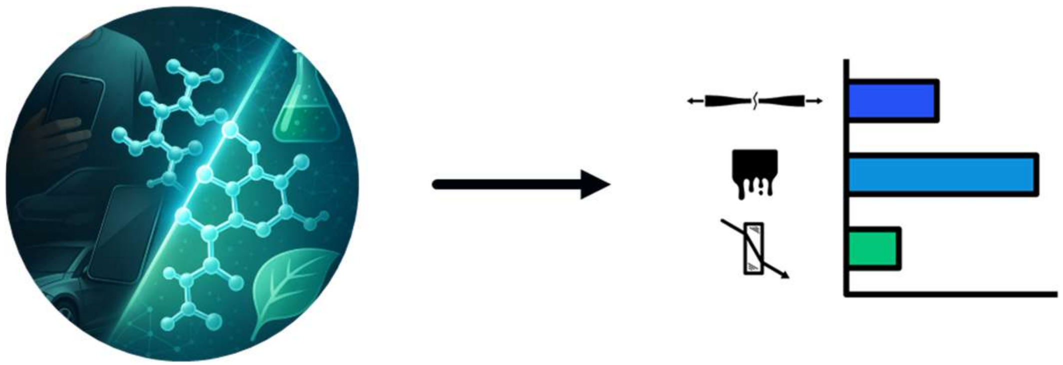
How to design new packaging materials with AI?

- polySCOUT has two modus of operandi: “forward design” & “inverse design”
- Forward: improve properties of existing polymers



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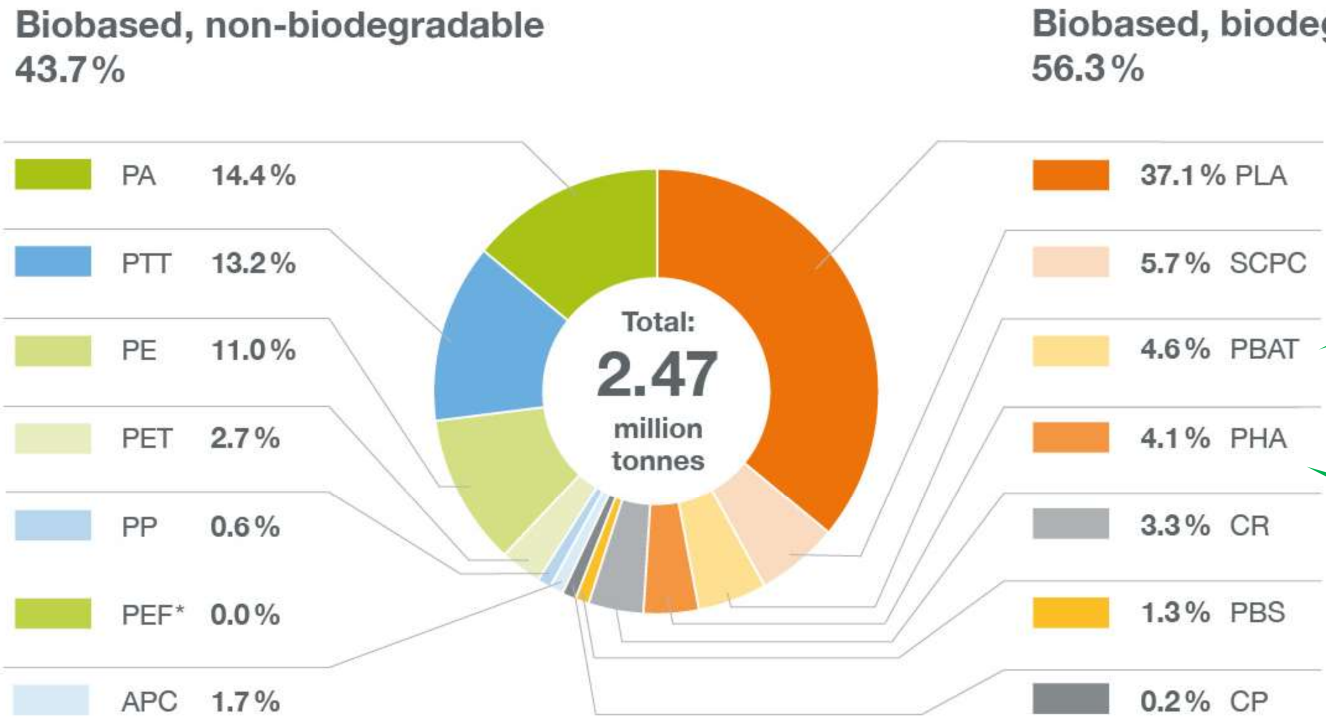

Use succinic versus adipic acid to improve sustainability & change properties

Generate blends or co-polymers of PHA with PLA, PGA or PEF

APC	Aliphatic Polycarbonates
CP	Casein Polymers
CR	Cellulose Regenerates
PA	Polyamides
PBAT	Poly(Butylene Adipate-co-Terephthalate)
PBS	Polybutylene Succinate and Copolymers
PE	Polyethylene
PEF	Polyethylene Furanoate
PET	Polyethylene Terephthalate
PHA	Polyhydroxyalkanoates
PLA	Polylactic Acid
PP	Polypropylene
PTT	Polytrimethylene Terephthalate
SCPC	Starch Containing Polymer Compounds

* PEF available at commercial scale as of 2024

Source: European Bioplastics, nova-Institute (2024)

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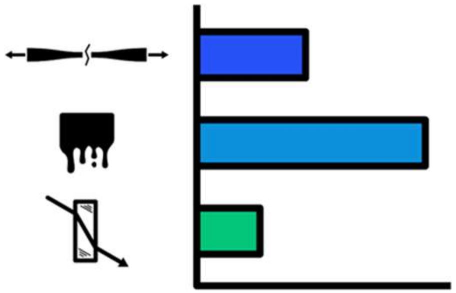
- Forward: improve properties of existing polymers
- Inverse: design (novel) polymer for target product



Plastic films need high elongation at break!

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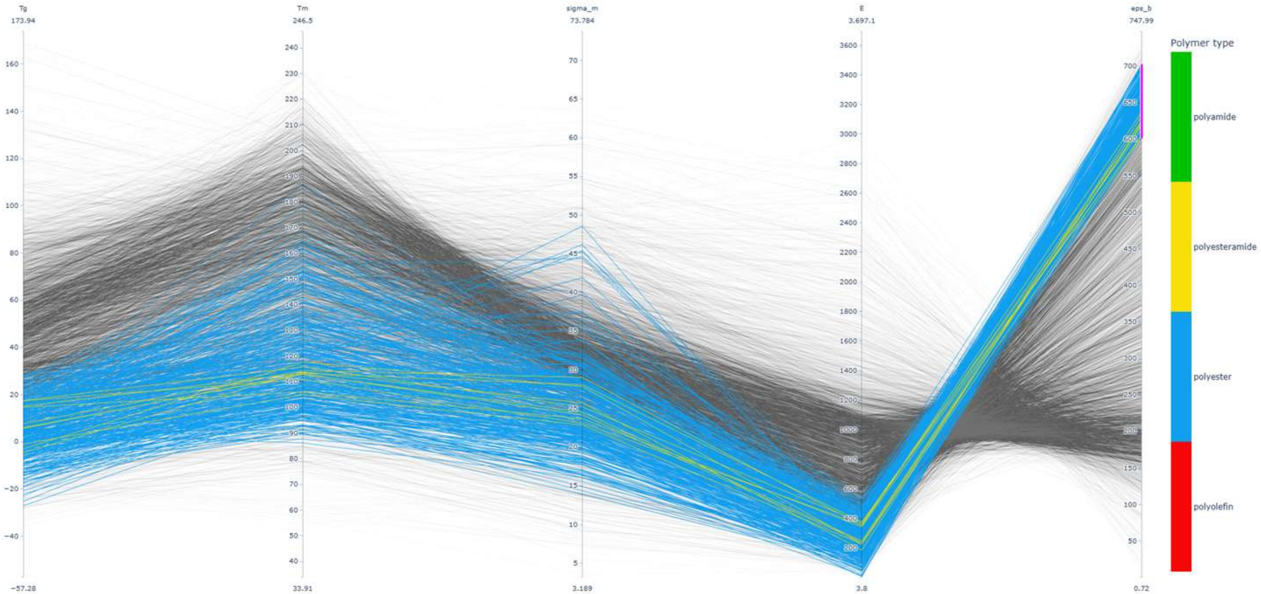
Potential options for polymers with high elongation at break



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Accelerating the transition to biobased, advanced polymeric materials for a sustainable future

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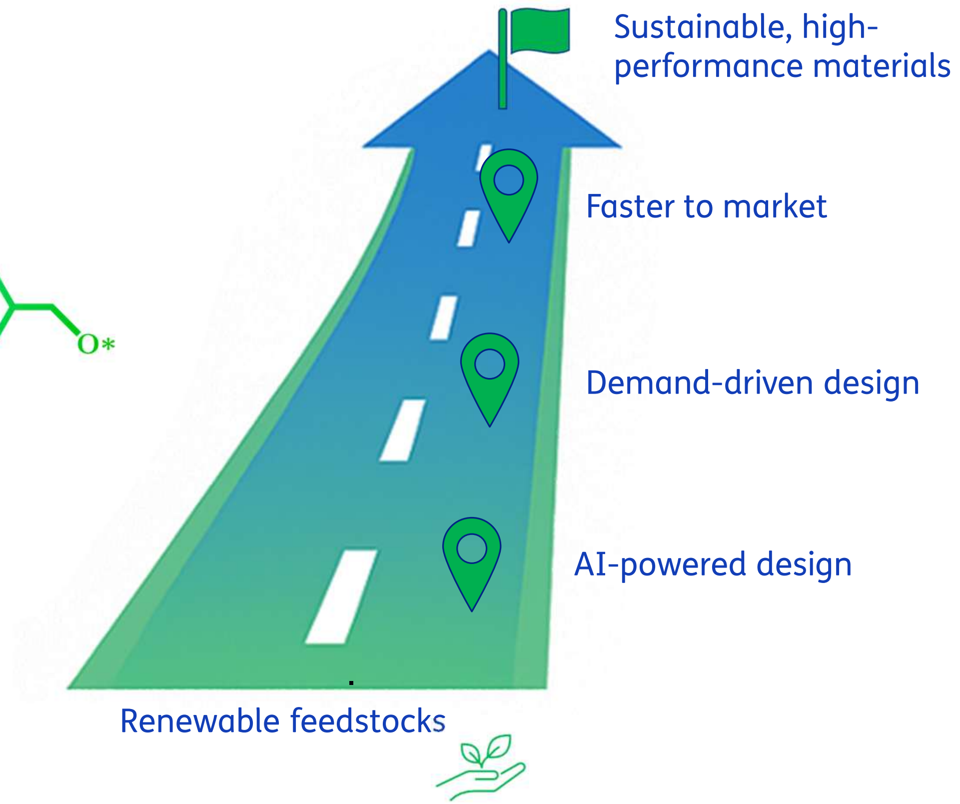
AI-powered & demand-driven polymer design

Partnerships for scale-up & application development



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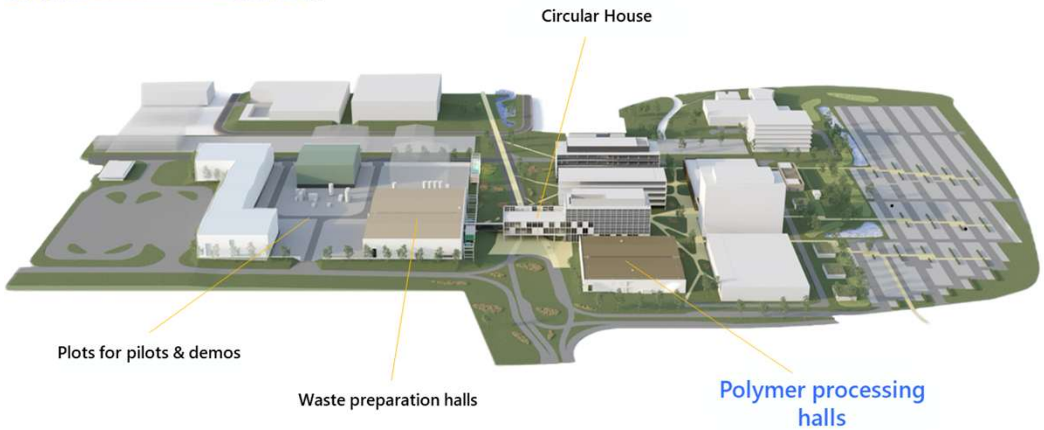
Brightlands Circular Space | application development

- Collaboration of TNO, Maastricht University & Brightlands Chemelot Campus
- Polymer powerhouse with facilities at lab & pilot-scale
- Key equipment: compounding line, cast/blown film & sheet line, bi-axial stretching + analysis



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Teamwork is the dreamwork!

Acknowledgement:
Dutch project BIOTTEK aims to develop new biopolyester with 6.6 million EUR investment

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Interested?

Please reach out to us →

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[Towards a circular economy: biopolymers by machine learning]