big chemistry

TNO innovation for life

# BigChemistry & TNO

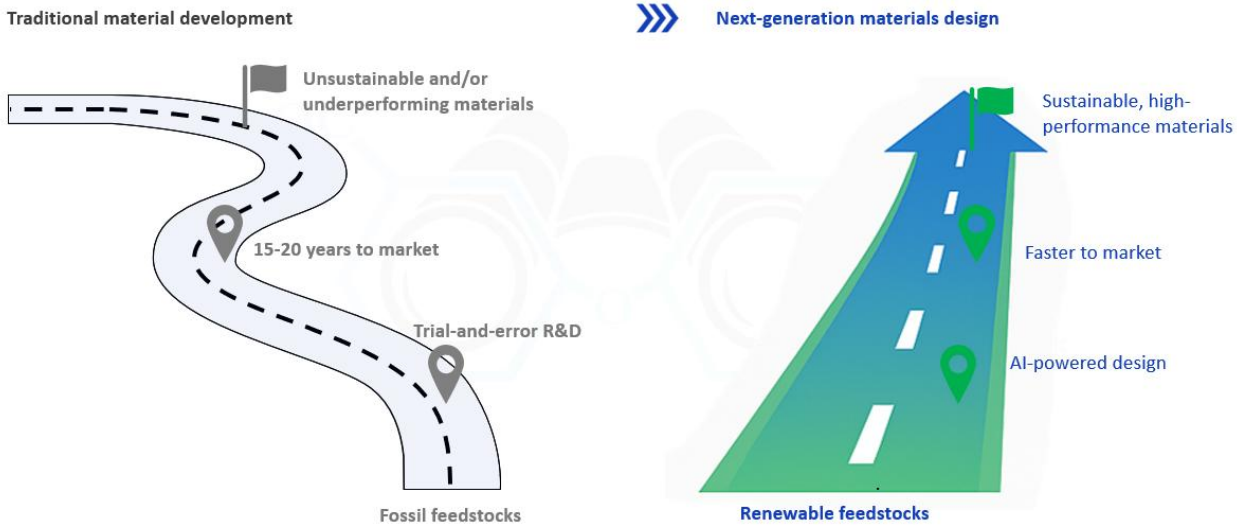
## An introduction on expertise and data driven formulation development &

## How could it support your company?

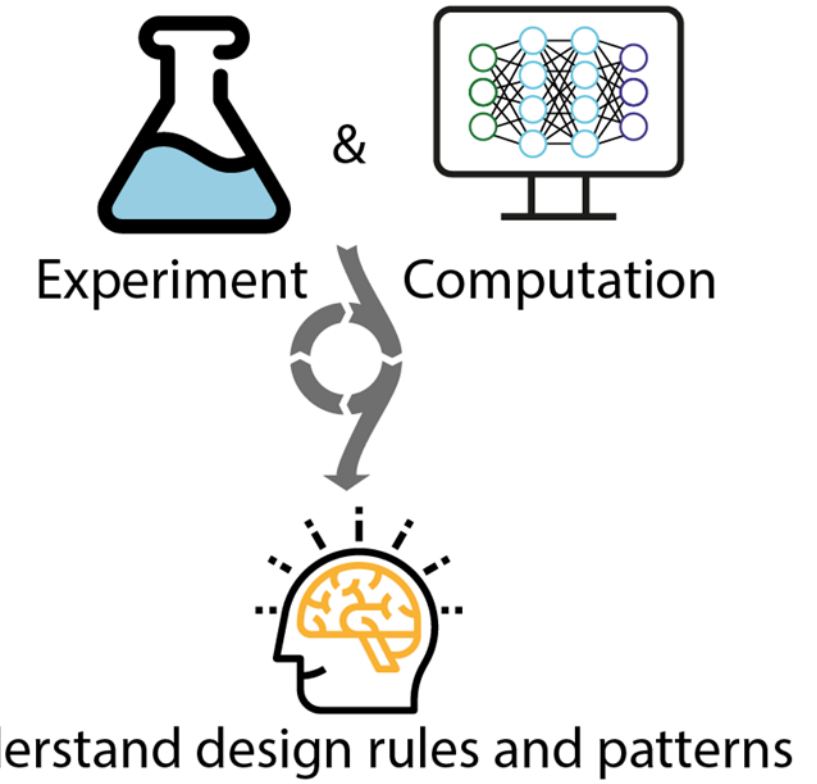
Pieter Imhof & Francesco Staps

**Both parties stand for accelerating the transition to sustainable, advanced formulations for an impactful future**

# TNO
# New ingredients




# Big Chemistry
# Formulation predictions



# Addressing Key Trends

- **Technological trend**: Electrification, Robotization and connectivity, zero (negative) carbon emission technologies, AI / ML.

- **Socio Economical**: The world is growing rapidly, and the population is aging. We need new sustainable and efficient ways to feed the world population. Products need to become more environmentally benign. Widening of the gap between rich and poor.

- **Regulatory trends**: GHG emission reductions, biodiversity, land and water use, phasing out the use of substances of concern such as fluorinated hydrocarbons (PFAS).

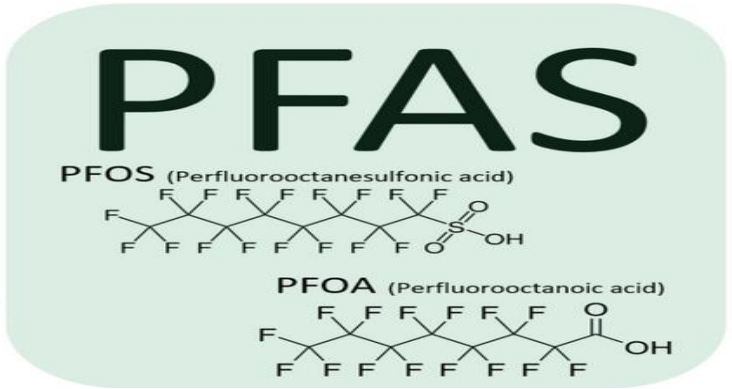
- **Cultural trends**: Climate issue is becoming more and more an issue among the public: sustainability becomes more important. Issues concerning health. Water quality and access to clean water issues.

# We live in a complex society, with complex problems


The **energy** transition also means a **materials** transition. Almost all materials around us were manufactured using materials from fossil sources.

We do not know how to replace those with alternative materials….

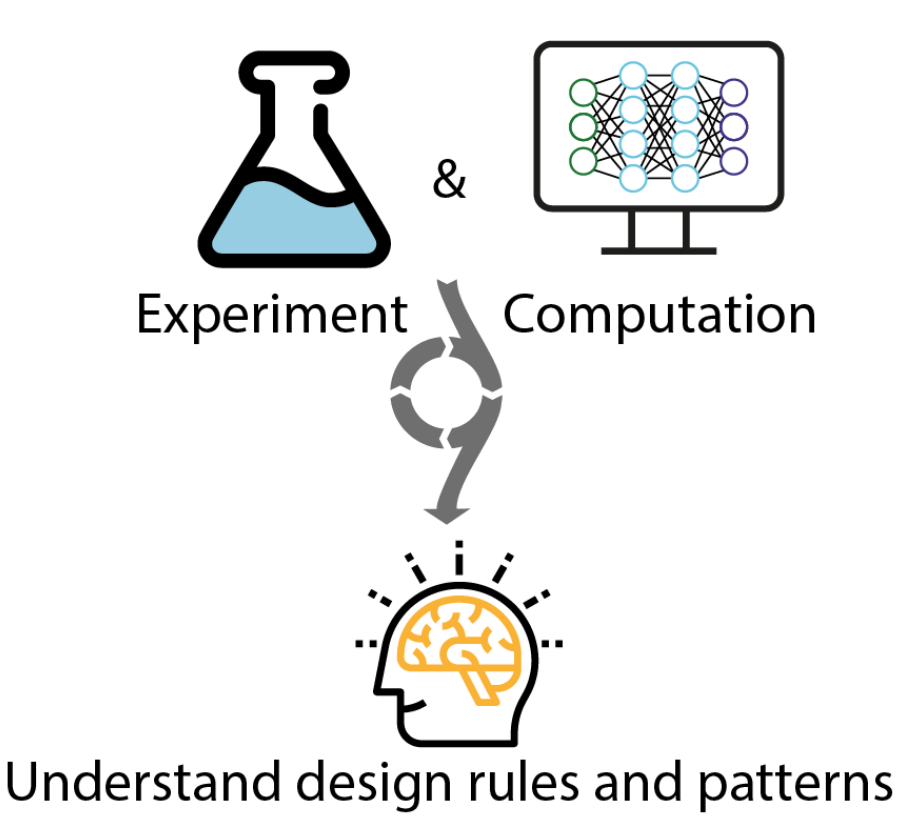
*Exchange ingredients to comply to (new) regulations*



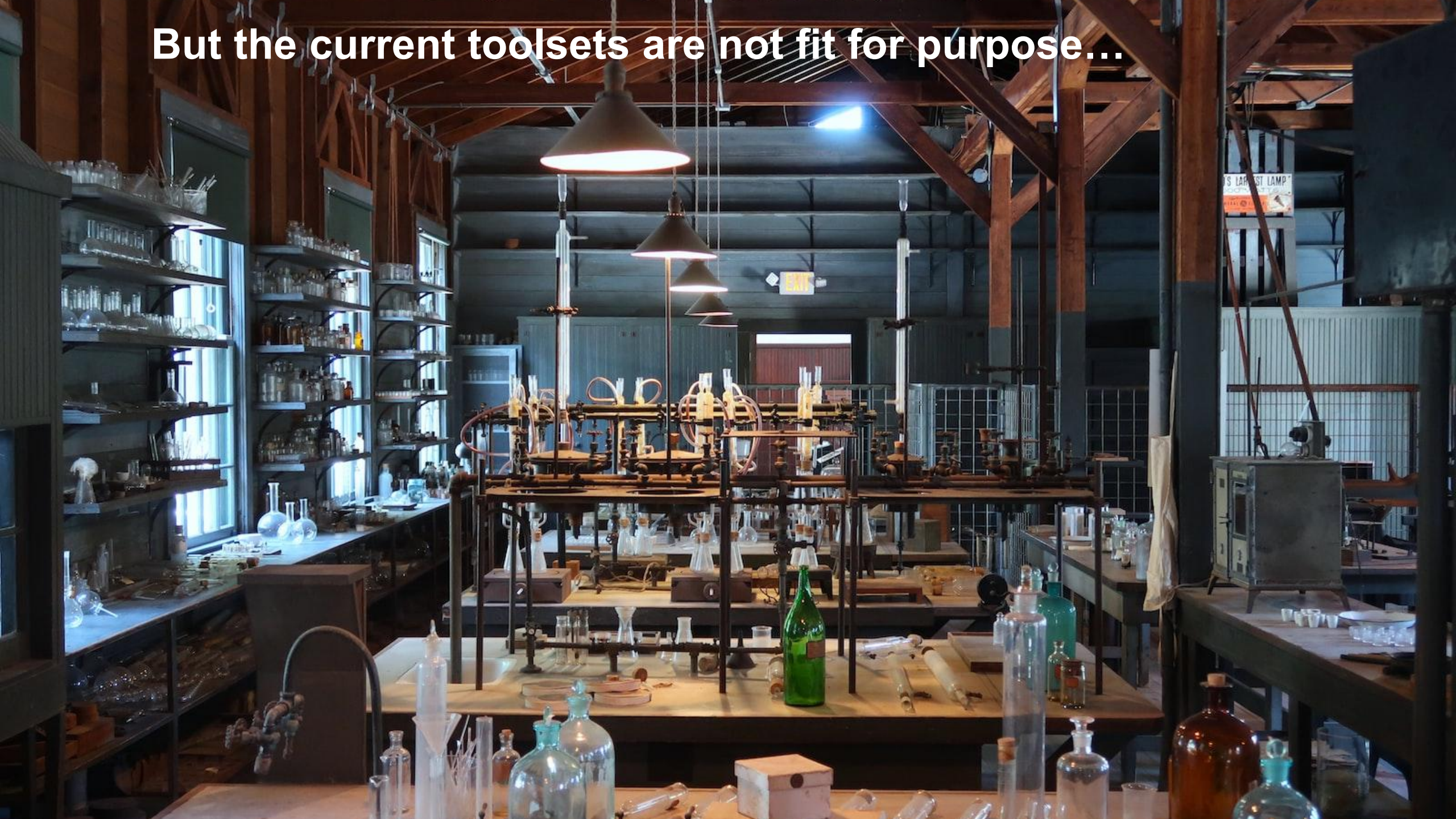

# The challenge

## “For chemists, the AI revolution has yet to happen.”*

- AI doesn’t (really) know chemistry…..
- AI needs **A LOT** of data (LargeLanguageModels were trained on billions of words),
- We need to know which data to use to train a model,
- Chemistry has a data problem – we need to use more of it in what we do!
- Big Chemistry already runs self-driving labs (robotic labs) to generate high quality data and will continue to do so!
- **The good news: chemistry and AI are a *perfect* match!**

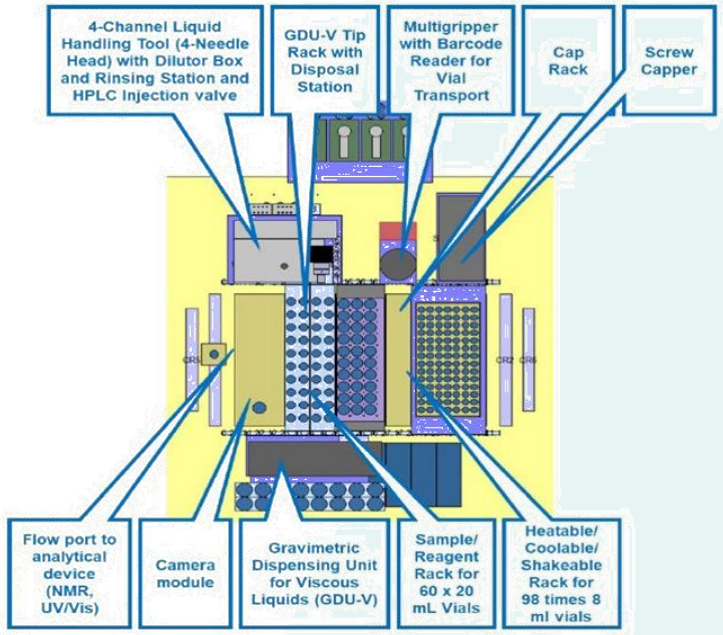



*Nature* 617, no. 7961 (18 May 2023): 438–438. https://doi.org/10.1038/d41586-023-01612-x.


But the current toolsets are not fit for purpose…

# Vision

- **Build large data sets and develop chemical AI models for physical and impact properties of molecular systems by integrating robotics and analytics.**
- **Aiming for improved formulations using existing and optional novel ingredients.**
- **Valorize existing data sets**




FLEX POWDERDOSE
Automated Workstation
L x W x H = 0.9 x 0.9 x 2.2 m

# Scientific Vision

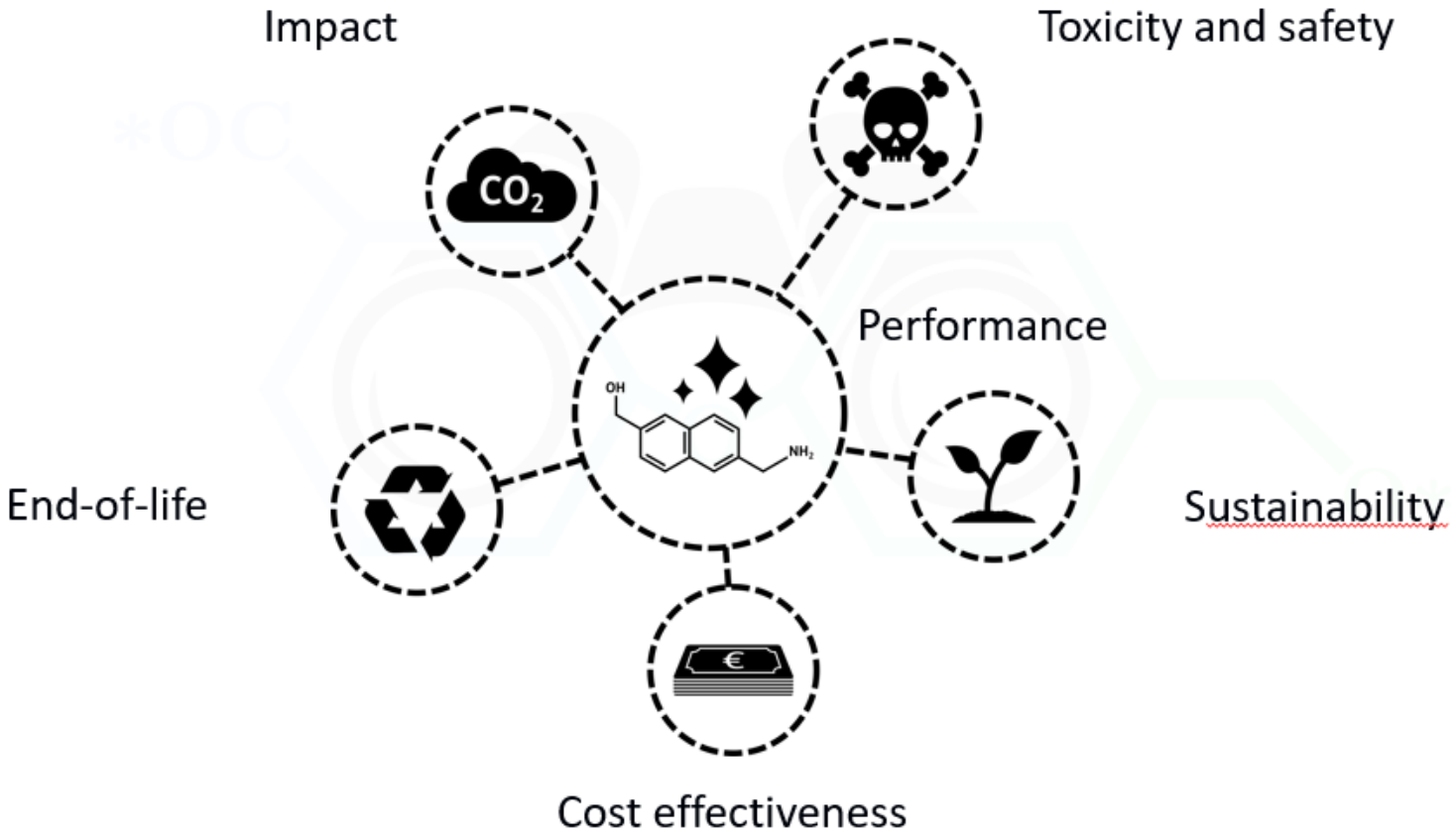
**Formulation: from an art to a science-based technology**

**Energy transition goes hand in hand with materials transition: we need to replace fossil-fuel derived ingredients**

- Properties emerge from the interactions between multiple components
- Focus on predicting physical properties of molecules (and mixtures)
- Build self-driving modules to generate data
- Exploit active learning algorithms, train predictive models

# Scientific Vision (cont'd)

## Addressing design parameters beyond properties



# The need for AI

Total number of molecules synthesized by chemist over last 100 years: **60 million**

Total number of molecules possible containing 17 atoms of C, N, O, S, and halogens: **166 billion**

The *chemical universe* is huge…. and we can never study every possible molecule.

**We need AI to search the chemical space and discover the most useful molecules (medicine, materials, energy, personal care, food, fragrance, paints, coatings, inks, etc.)**

# Big Chemistry Consortium

"…chemical **AI** and build **large data sets** on **physical properties** of molecular systems by integrating **robotics** and analytics."

"…develop the RobotLab as a **commercial international entity**"

We have 97M Euros and 7 years…. **(start July 2023**)

5 partners:

Universities: Eindhoven, Groningen, Nijmegen

University of Applied Sciences: Fontys

Research Institute: AMOLF


Nationaal Groeifonds

# Benefitting from expertise and data driven approach

## Who

### Ink & coating producers:

- Shorter time to market for your formulations
- Right fit between formulation and application
- Sustainable ingredients

### Brand owners:

- Sustainable products fully meeting your customers need & requirements
- Replacing fossil based, traditional products

### Scientists:

- Supporting your expertise with structure – ratio – property predictions
- Accelerate innovation

## Collaborate:

- Join expert teams of Big Chemistry & TNO
- Maximizing synergy in
  - AI
  - High Throughput expertise
  - Material and formulation expertise

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# Benefitting from expertise and data driven approach

## How

### Data search, creation and validation:

- Literature
- High throughput syntheses, formulation, characterization & validation

### Develop Hybrid SPFs (Structure-Property Functions)

- Hybrid fingerprinting techniques
- Machine learning for resin & formulation prediction

### Formulation Design:

- Development of resin & formulation models
- Generate products with desired properties
- Including sustainability, safety & techno-economic properties

### Validate & Demonstrate:

- Formulate & characterize predicted candidates
- Incorporate findings in models

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# In summary ….

- Acceleration: The quest to Ink & Coatings formulation design can become an overnight activity
- Support formulating your novel products by assessing the viability of the production
  1. Sustainability impact
  2. Availability of ingredients
  3. Cost
  4. Safety and health
  5. Lower risks



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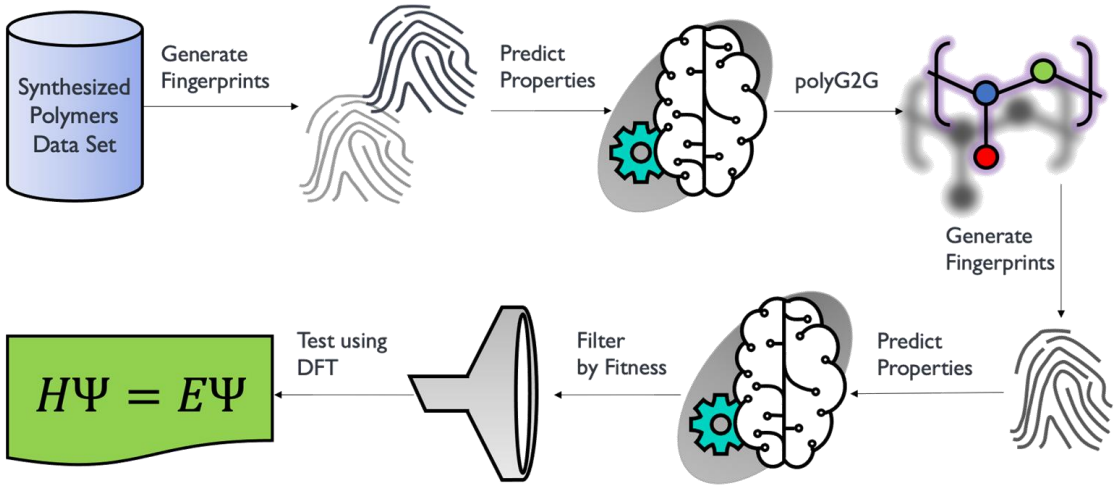
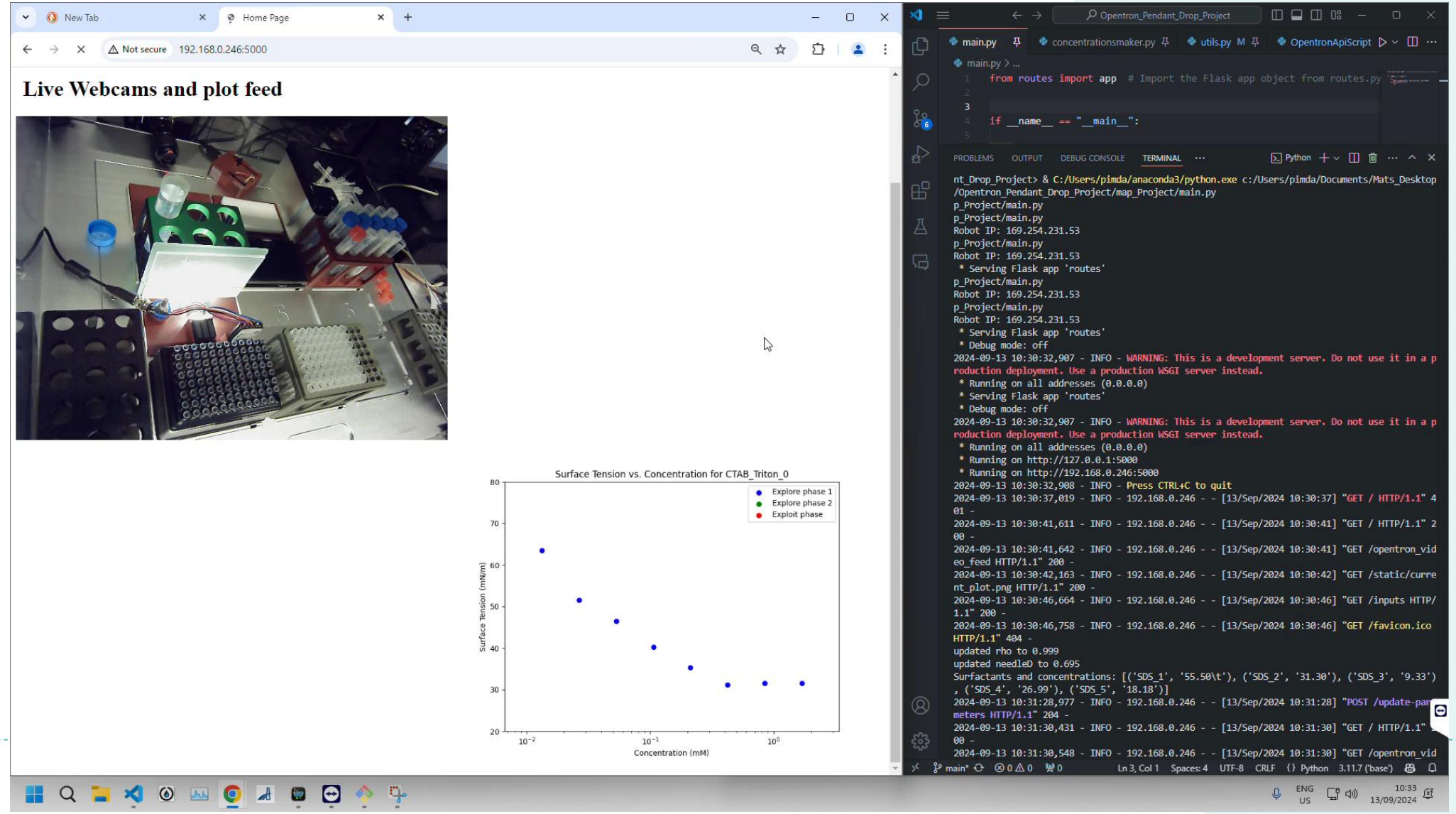
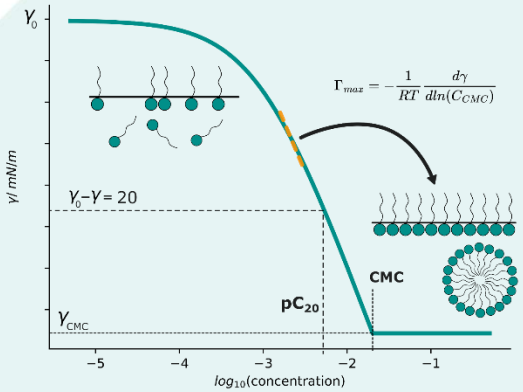
- Deliver on your promises: Quality, Innovation, Costs
- Enhance expert & data driven solutions

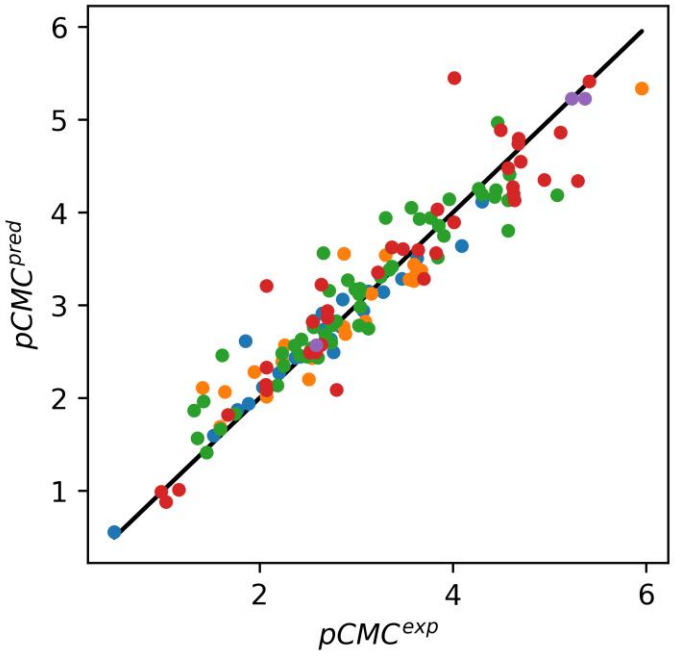


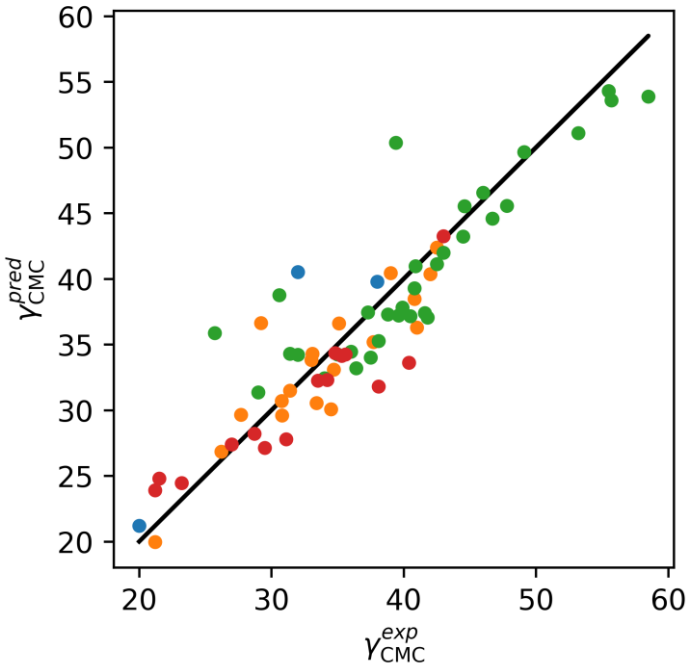
# ‘Live’ Demonstration

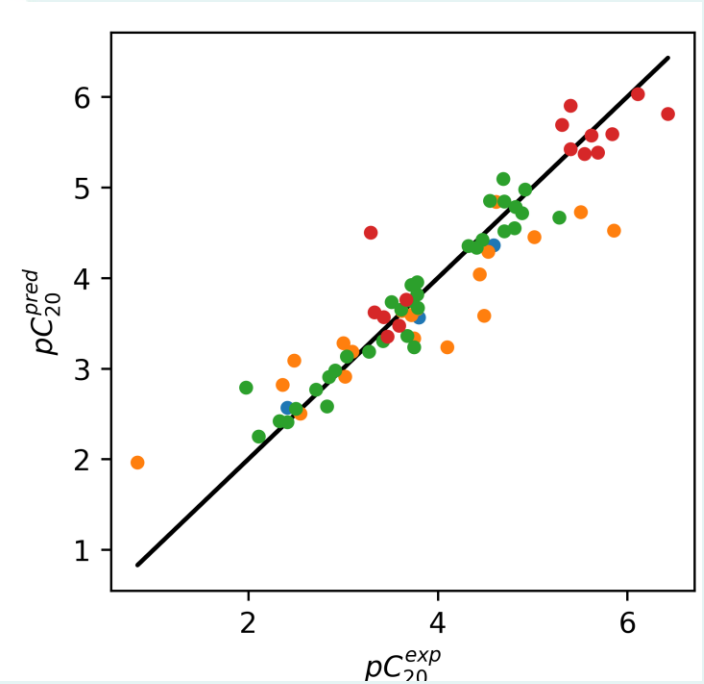


# An example:
# ML trained to predict surfactant properties



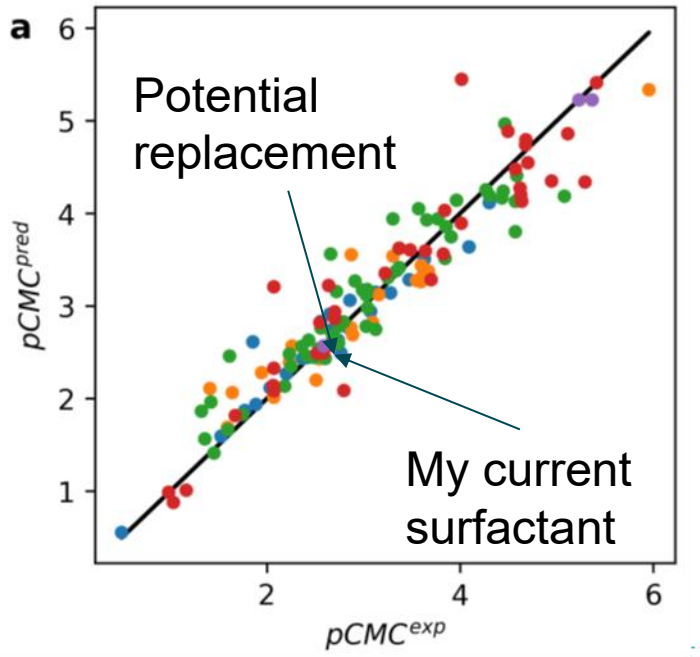

Accurate prediction of *all* properties of *all* 1600 surfactants: saves 1000's of hours of experimental work!!!

*Digital Discovery* **2025**, revision submitted

# How does that support your objectives?

Currently

Assuming you want/need to replace a surfactant




Future (approx 5 years)

Q: “Hey Robolab, my current formulation contains ingredients A/B/C etc at levels K/L/M % etc with water as dilutant.
If I want to replace ingredient C whilst upholding all performance and characteristics (specified) AND the cost price per MT cannot increase over 5%, what are my alternatives?”

A: Replace M% of ingredient C with 1,2*M of ingredient AA from supplier 5 or consider 1,6*M of ingredient BB from supplier 11.

# How can we support & cooperate?

In many ways

- given the fact that more than 50 PhD students and postdocs are working on the Big Chemistry project!
  - Having access to relevant knowledge and knowledgeable professors.
  - Running the self-driving, robotized high throughput set ups that are owned by Big Chemistry.

- Is there a preferred area to cooperate?

# Interested? Please reach out to us

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