



POLYMAT



## Agenda – Machine Learning for Polymer Science

### Day 1 – 8 June 2026

- 09:00 – 10:00 Usue Mori (University of the Basque Country)  
An Introduction to Machine Learning
- 10:00 – 11:00 Gustavo Schwartz (Centro de Física de Materiales)  
New approaches to addressing data scarcity and molecular representation for predicting polymer properties with neural networks
- 11:00 – 11:30 ☕ Coffee Break
- 11:30 – 12:30 Matthias Hermann (Citrine Informatics)  
Accelerating Material and Product Development through AI
- 12:30 – 13:30 Alfred Bazin (Arkema)  
Modeling and innovation in Arkema: From small molecules to materials

### Day 2 – 9 June 2026

- 09:00 – 10:00 Sabine Beuermann (Clausthal University of Technology)  
Modeling and reverse engineering of polymerizations based on KI and machine learning methods
- 10:00 – 11:00 Maciej Haranczyk (IMDEA Materials Institute)  
Towards self-driving polymer laboratory
- 11:00 – 11:30 ☕ Coffee Break
- 11:30 – 12:30 Gregor Simm (Microsoft Research)  
Simulation of Polymers with Machine Learning Force Fields
- 12:30 – 13:30 Thomas Nevolianis (Covestro)  
Digital Polymer Science in Practice: Use Cases from Industry

In collaboration with:



# Course: Machine Learning for Polymer Science

8-9 JUNE 2026

9:00 - 13:30

Miramar Palace  
San Sebastian

## Invited Lectures



**Alfred  
Bazin**

ARKEMA



**Sabine  
Beuermann**

CLAUSTHAL UNI.  
OF TECHNOLOGY



**Maciej  
Haranczyk**

IMDEA MATERIALS



**Matthias  
Hermann**

CITRINE  
INFORMATICS



**Usue  
Mori**

BCAM  
EHU



**Thomas  
Nevolianis**

COVESTRO



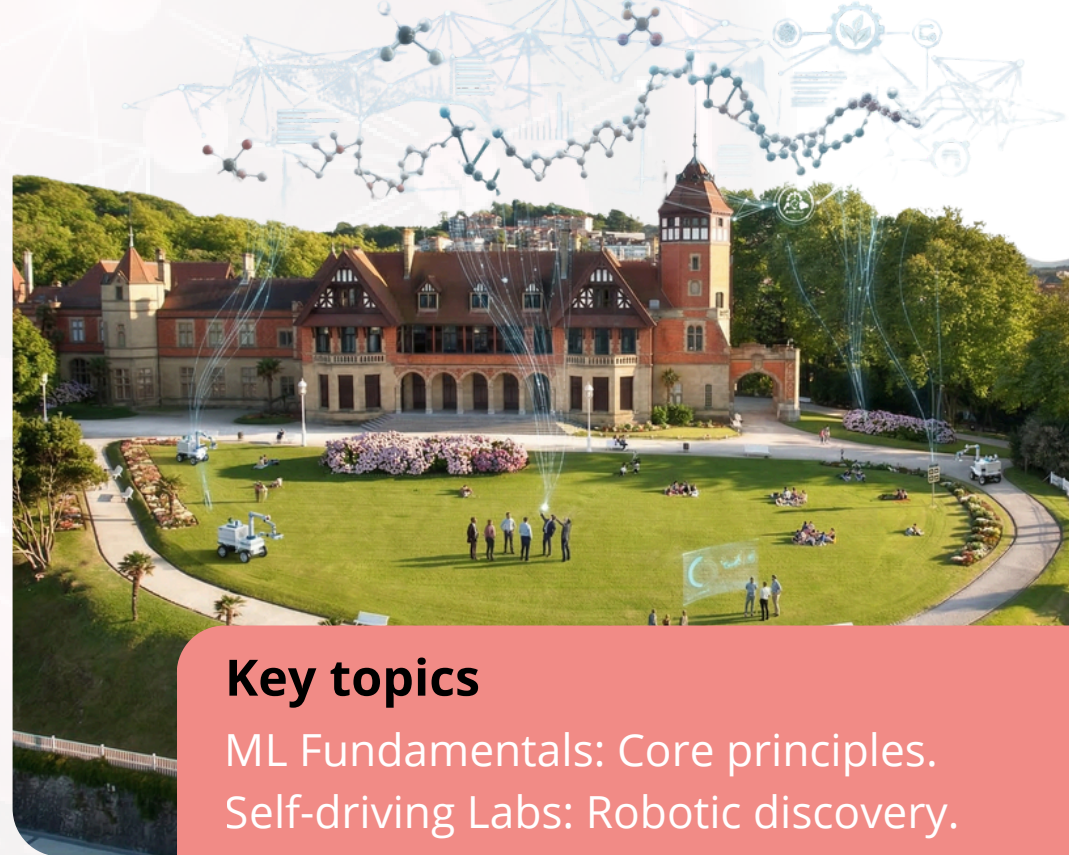
**Gregor  
Simm**

MICROSOFT  
RESEARCH



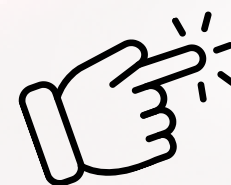
**Gustavo A.  
Schwartz**

CFM  
CSIC



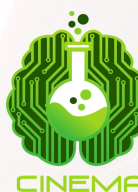
### Key topics

ML Fundamentals: Core principles.  
Self-driving Labs: Robotic discovery.  
Polymer Simulation: AI-aided modeling.  
Digital R&D: Industrial applications.



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**Fee: 100€**



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