Machine Learning for Polymer Science

08.juin - 09.juin 2026

Cod. Z55-26

Modalité:
En personne

Édition
2026

Type d'activité
Workshop

Date
08.juin - 09.juin 2026

Location
Miramar Palace

Langues
Anglais

Reconnaissance officielle par l'État
20 heures

Comité d'organisation

Description

San Sebastian will host the course *“Machine Learning for Polymer Science”*, bringing together researchers working at the intersection of **machine learning, polymer science and materials research**.

The school aims to provide a comprehensive overview of how **data-driven approaches and artificial intelligence are transforming polymer science**, offering a unique opportunity to bridge **fundamental concepts with real-world applications** in both academic and industrial contexts.

The programme will cover key topics including:

- **Fundamentals of machine learning and data-driven modeling**
- **Self-driving laboratories and autonomous experimentation**
- **Machine learning assisted simulation of polymers and polymerization processes**
- **Digital R&D and industrial applications in polymer science**
- **Sustainable materials design through AI approaches**

The course will include lectures from leading experts in academia and industry, providing participants with both **theoretical foundations and practical insights** into the implementation of machine learning tools. The school aims to enable attendees to apply machine learning techniques in their own research and contribute to the development of **intelligent and sustainable materials for the future**.

INVITED LECTURERS

- Alfred Bazin (Arkema)
- Gregor Simm (Microsoft Research)
- Maciej Haranczyk (IMDEA Materials Institute)
- Thomas Nevolianis (Covestro)
- Matthias Hermann (Citrine Informatics)
- Sabine Beuermann (Clausthal University of Technology)
- Usue Mori (University of the Basque Country EHU and BCAM)

Objectifs

To promote the exchange of knowledge between researchers working at the interface of **machine learning, polymer science and materials research**.

To present the **latest advances in data-driven materials science**, including machine learning fundamentals, polymer simulation, self-driving laboratories and digital R&D approaches.

To provide participants with both **theoretical foundations and practical insights** into the application of artificial intelligence in polymer science.

To foster the **active participation of early-career researchers** through discussions and interaction with leading experts from academia and industry.

To strengthen the connection between **academic research and industrial innovation**, showcasing real use cases of machine learning in polymer development.

To contribute to the development of a **scientific community skilled in digital and sustainable approaches**, addressing current challenges in materials design and innovation.

Organisée par

En collaboration avec

Directed by

Nicholas Ballard

Polymat - University of the Basque Country

Nicholas Ballard is an Ikerbasque Associate Professor at POLYMAT specialized in polymer chemistry, reaction engineering, and advanced polymerization processes, with a strong focus on data-driven approaches and machine learning applied to materials science. His research combines fundamental understanding of polymerization kinetics with the development of sustainable and efficient polymer production processes. He has extensive experience in European research projects, including coordination and participation in Horizon Europe and MSCA programmes, and plays a key role in international collaborative networks. His work has resulted in numerous high-impact scientific publications and contributions to the advancement of bio-based polymers and smart materials. At POLYMAT, he leads research activities related to polymerization modeling and process optimization, contributing to interdisciplinary projects at the interface of chemistry, engineering, and artificial intelligence.

Mónica Moreno Rodríguez

Basque Center for Macromolecular Design and Engineering

Mónica Moreno is Head of the Project Office at POLYMAT. She holds a PhD in Chemistry and has solid expertise in the management of European research projects, particularly within Horizon Europe and MSCA programmes. She specializes in project coordination, financial and administrative management, and liaison with the European Commission, supporting the successful implementation of international collaborative research initiatives.

Professeurs

Alfred Bazin

Alfred Bazin studied Chemistry and Polymer Science in Strasbourg, where he later completed a PhD at ICPEES focused on the synthesis and characterization of biobased polymers. After his doctorate, he specialized in machine learning with a particular emphasis on applications in polymer science. He is currently part of Arkema’s R&D Digital team, working as a Data Scientist and Digital Acculturation Scientist, where he advances data-driven approaches in R&D and leads initiatives to promote digital awareness and adoption across the organization.

Sabine Beuermann

Maciej Haranczyk

Maciej Haranczyk received his PhD in Chemistry from the University of Gdańsk (Poland) in 2008. During his doctoral studies, he held several international research fellowships and collaborated with leading institutions, including Pacific Northwest National Laboratory, the University of Southern California, and the University of Sheffield. After his PhD, he joined Lawrence Berkeley National Laboratory as a Glenn T. Seaborg Postdoctoral Fellow, later becoming a Research Scientist and subsequently a Staff Scientist. In 2015, he joined IMDEA Materials Institute as a Senior Researcher under the Ramón y Cajal programme. He currently leads the Accelerated Materials Discovery Group and manages a robot-equipped polymer research laboratory focused on data-driven approaches for materials design.

Matthias Hermann

Matthias Hermann is a Senior Solutions Engineer at Citrine Informatics. He holds a PhD in Analytical Chemistry from Queen’s University, where he focused on the development of microfluidic devices for automated mass spectrometry. He also has industrial experience as a lab team leader at BASF, where he led high-throughput screening projects for polymer formulations.

Usue Mori Carrascal

Unviersidad del Pais Vasco. EHU

Usue Mori obtained a Bachelors degree in Mathematics and a PhD in Computer Engineering from the University of Basque Country UPV/EHU in 2010 and 2015 respectively. She completed a master's degree in Applied Mathematics, Statistics and Computing and a master's degree in Computer Engineering and Intelligent Systems in 2011 and 2013, respectively. Currently, she is an associate professor in the Department of Computer Science and Artificial Intelligence at the University of the Basque Country UPV/EHU and teaches various subjects in the field of mathematics, statistics and machine learning. As research merits, it should be noted that she has participated in more than 20 projects of regional, state and European calls, being IP in four of these projects. She has published 18 articles in JCR journals, 12 of them located in the first quartile and she also has 4 contributions in national and international conferences. She has also participated in 6 R&D contracts with companies of the private industrial and public sector, being IP the most recent. In addition, she has co-directed two doctoral theses and today she co-directs 3 doctoral theses with other researchers.

Thomas Nevolianis

Thomas Nevolianis is a Cheminformatics Expert at Covestro’s Digital Research and Development in Leverkusen, Germany, where he supports R&D projects across the company’s global operations. He obtained his PhD in Chemical Engineering from RWTH Aachen University, following undergraduate studies in Physics. During his doctoral research, he held a visiting scholarship at MIT, specializing in molecular property prediction using machine learning and quantum chemical methods. At Covestro, his work focuses on computational approaches to polymer development, including the screening of

monomers and additives for next-generation materials, prediction of polymer–solvent compatibility, and optimization of formulations. His research integrates graph neural networks, machine learning interatomic potentials, quantum mechanics, and molecular dynamics simulations to address regulatory, sustainability, and performance challenges. By translating computational methods into practical workflows, he contributes to accelerating materials discovery while reducing experimental time and costs.

Gregor Simm

Gregor Simm is a Senior Researcher and Project Lead at Microsoft Research, working within the AI for Science initiative. His research focuses on machine learning and atomistic simulation of matter, with strong interests in geometric deep learning, reinforcement learning, and generative modelling. From 2018 to 2021, he was a Research Associate in the Machine Learning Group at the University of Cambridge. He obtained his PhD in Theoretical Chemistry from ETH Zurich (2015–2018).

Tarifs inscription

INSCRIPTION	JUSQU'AU 01-06-2026
Général	100,00 EUR

Lieu

Miramar Palace

Pº de Miraconcha nº 48. Donostia / San Sebastián

Gipuzkoa