EUPOC 2026

Designing New Polymers by Combining High-Throughput and Artificial Intelligence Tool

May 18-21, 2026 - Bertinoro (FC), Italy

Chairs

D. Grande
Universitè de Strasbourg

J.F. Gérard
Universitè de Lyon

M. Laus
Università del Piemonte Orientale

S. Pruvost
INSA Lyon

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Program

Conference Program Overview

Monday, 18 May 2026 SALA RAVELLINO		
13:45-14:45		**Light Lunch***
14:45-15:45		**Registration**
15:45-16:00		**Opening**
Session A: Chair: Jean-François Gerard		
16:00-16:45	**PL1**	**Arthi JAYARAMAN, USA** *Molecular modeling, simulations, and machine learning to solve polymer science problems from industry*
16:45-17:30	**PL2**	**Kevin Maik JABLONKA, Germany** *Patterns, Predictions and Actions for Material Design*
17:30-17:50	**OC1**	**Amaia ELIZARAN MENDARTE, Spain** *Similarity-driven framework for few-shot data-efficient polymer property prediction*
19:00-21:30		**Welcome Party****

PL = Plenary Lecture (40 min + 5 min discussion)

OC = Oral Communication (15 min + 5 min discussion)

*@The Terrace above Sala Ravellino

**@the Fortress's Terrace

Conference Program Overview (contd.)

Tuesday, 19 May 2026 (morning) SALA RAVELLINO		
08:30-09:00		Registration
Session B, Chair: Arthi JAYARAMAN		
09:00-09:45	**PL3**	**Federico FERRARESE LUPI, Italy** *Data-driven design of block copolymer self-assembly*
09:45-10:05	**OC2**	**Hiba HAMMOUD, France** *Study and simulation of photopolymerization reaction*
10:05-10:25	**OC3**	**Hamid ZENTOU, Saudi Arabia** *Practical prediction of gas separation performance in polymeric membranes using machine learning*
10:25-11:00		**Coffee Break**
11 :00-11:45	**PL4**	**Andrea GIUNTOLI, Netherlands** *Adding physics to AI for efficient-throughput Molecular Dynamics*
11:45-12:30	**PL5**	**Giuseppe MILANO, Italy** *From hybrid particle-field MD to machine learning: density fields as physics-informed representations for polymer design*
12:30-13:05	**OC4**	**Ivana SEDENKOVA, CZ** *Heterospectral machine learning for structural analysis of alginate–pectin networks: correlating distinct spectroscopic modalitie*
13:05-14:30		**Lunch**

PL = Plenary Lecture (40 min + 5 min discussion)

OC = Oral Communication (15 min + 5 min discussion)

Conference Program Overview (contd.)

Tuesday, 19 May 2026 (afternoon) SALA RAVELLINO		
Session C, Chair: Michele Laus		
14:30-15:15	**PL6**	**Simon HARRISSON, France** *Data-Driven Polymerization In Flow: Machine Learning Strategies For Accelerated Polymer Discovery*
15:15-16:00	**PL7**	**Michele Perego, Italy** *Innovative Hardware and Alternative Algorithms for Unconventional Computing at the Edge*
16:00-16:20	**OC5**	**Emelia GRIFFITHS, UK** *Development of an automated reactor platform for the synthesis of functional polymers*
16:20-16:40	**OC6**	**Jonathan GUILD, UK** *Synthesis of homo- and gradient co-polymers via Living Anionic Polymerisation within a continuous flow reactor*
16:40-17:00		Coffee Break
Session D, Chair: Marian Scuturici		
17:00-17:45	**PL8**	**Alexis BIGO-SIMON, France** *Cryo-EM & AI: On the road to structure discovery*
17:45-18:05	**OC7**	**Emily DIXON, UK** *D-Optimal design for enzymatic ring-opening polymerization of e-Caprolactone toward sustainable polyester synthesis using biobased solvents*
18:15-19:15		***POSTER SESSION with WINE*****

PL = Plenary Lecture (40 min + 5 min discussion)

OC = Oral Communication (15 min + 5 min discussion)

**@Calligari – 1st Floor Fortress

Conference Program Overview (contd.)

Wednesday, 20 May 2026 (morning) SALA RAVELLINO		
Session E, Chair: Simon Harrisson		
09:00-09:45	**PL9**	**Marian SCUTURICI, France** *Leveraging artificial intelligence for materials discovery: opportunities and challenges*
09:45-10:30	**PL10**	**Patrick RINKE, Germany** *AI-guided optimization and characterization of lignin*
10:30-10:50	**OC8**	**Aymar Lebeau TCHAGOUE, France** *AI for polymer design: multi-score reinforcement learning for HighTg polyimide discovery*
10:50-11:15		**Coffee Break**
Session F, Chair: Daniel Grande		
11:15-12:00	**PL11**	**Ulrich S. SCHUBERT, Germany** *High-throughput experimentation for polymers: from quantitative structure-property relationships towards application of machine-learning*
12:00-12:20	**OC9**	**Maxwell TERBAN, Germany** *From molecules to morphology: high-throughput X-ray scattering for multi-length-scale characterisation of polymer structures*
12:20-12:40	**OC10**	**Laura MISRACHI, France** Synboli: Accelerating the development of high performance polymer materials through AI
13:00-14:30		**Lunch**
17:00		**SOCIAL EVENT** *Wine tasting hosted in Bertinoro municipal hall*
20:00		**Conference Dinner***

PL = Plenary Lecture (40 min + 5 min discussion)

OC = Oral Communication (15 min + 5 min discussion)

*@Ca' de Bè Osteria Enoteca

Conference Program Overview (contd.)

Thursday, 21 May 2026 (morning) Sala Ravellino		
Session G, Chair: Sébastien Pruvost		
9:00-9:45	**PL12**	**Khalid FERJI, France** *Machine learning for multiscale polymer systems*
9:45-10:30	**PL13**	**Nicholas BALLARD, Spain** *Knowledge guided machine learning for polymer science*
10:30-11:00		**Coffee Break**
11:00-11:20	**OC11**	**Francesco CATALINI, Italy** *Development of nanofiltration hybrid membranes for sustainable heterogeneous catalysis in continuous-flow*
11:20-11:40	**OC12**	**Eleonora RICCI, UK** ***Screening polymers for gas separations with a hybrid physics-based and Data Driven Strategy***
11:40-12:00		**Prizes Awarding & Final Remarks**
13:15		**Shuttle Departure to Bologna Airport and Bologna Railway Station**

PL = Plenary Lecture (40 min + 5 min discussion)

OC = Oral Communication (15 min + 10 min discussion)

Conference Program

Monday, 18 May 2026

13.45-14:45 Light Lunch *@The Terrace above Sala Ravellino*

14:45-15:45 Registration

15:45-16:00 Opening

Session A

Chairman: *Jean-François Gerard*

16:00-16:45 **PL1** **A. Jayaraman**
University of Delaware (USA)
Molecular modeling, simulations, and machine learning to solve polymer science problems from industry

16:45-17:30 **PL2** **K.M. Jablonka**
Friedrich Schiller University Jena (Germany)
Patterns, prediction and actions for Material Design

17:30-17:50 **OC1** **A. Elizaran-Mendarte**, G. A. Schwartz
CFM – CSIC/EHU (Spain)
Similarity-driven framework for few-shot data-efficient polymer property prediction

19:00-21:30 **Welcome Party @the Fortress's Terrace**

Tuesday, 19 May 2026 (morning session)

08:30-09:00 Registration

Session B
Chairman: *Arthi Jayaraman*

09:00-09.45 **PL3** **F. Ferrarese Lupi**
INRiM (Italy)
Data-driven design of block copolymer self-assembly

09:45-10:05 **OC2** **H. Hammoud,** C. Dietlin, A. Hijazi, J. Lalevée
Université de Haute-Alsace (France)
Study and simulation of photopolymerization reaction

10:05-10:25 OC3 **H. Zentou**
King Fahd University of Petroleum and Minerals – KFUPM, (SA)
Practical prediction of gas separation performance in polymeric membranes using machine learning

10:25-11:00 **Coffee Break**

11:00-11:45 **PL4** **A. Giuntoli**
University of Groningen (NL)
Adding physics to AI for efficient-throughput molecular dynamics

11:45-12:30 **PL5** **G. Milano,** J. Shi, T. Sui, J. Wu, S. Liu, Y. Wang, S. Lin, S. Xu, M. He, J. Mao, G. Zhang, Y. Zha
University of Naples "Federico II" (Italy)
From hybrid particle-field molecular dynamics to machine learning: density fields as physics-informed representations for polymer design

12:30-13:05 **OC4** **I. Sedenkova**, M. Urbanova. J. Brus
Institute of Macromolecular Chemistry CAS, (CZ)
Heterospectral machine learning for structural analysis of alginate–pectin networks: correlating distinct spectroscopic modalities

13:05-14:30 **Lunch**

Tuesday, 19 May 2026 (afternoon session)

Session C
Chairman: *Michele Laus*

14:30-15:15 **PL6** **S. Harrisson**
Université de Bordeaux (FR)
Data-driven polymerization in flow: machine learning strategies for accelerated polymer discovery

15:15-16:00 **PL7** **M. Perego**
CNR-IMM (IT)
Innovative hardware and alternative algorithms for unconventional computing at the edge

16:00-16:20 **OC5** **E. Griffiths**, N. Kapur, R.A. Bourne, A.D. Clayton, N.J. Warren
University of Leeds (UK)
Development of an automated reactor platform for the synthesis of functional polymers

16:20-16:40 **OC6** **J.D. GUILD**, N. Kapur, R.A. Bourne, N.J. Warren
University of Sheffield (UK)
Continuous flow living anionic polymerization for the one-step synthesis of block-like copolymers

16:40-17:00 **Coffee Break**

Session D
Chairman: *Marian Scuturici*

17:00-17:45 **PL8** **A. Bigo-Simon**
ECPM Strasbourg (FR)
Cryo-EM & AI: on the road to structure discovery

17:45-18:05 **OC7** **E.G. Dixon**, E. Chau, L. Ciano, A. Pordea, K. Alvey, V. Taresco
University of Nottingham (UK)
D-optimal design for enzymatic ring-opening polymerization of ε-CaprolactoneL toward sustainable polyester synthesis using biobased solvents

18:15-19:15 **Poster session and wine @Calligari – 1st Floor Fortress**

Wednesday, 20 May 2026 (morning session)

Session E
Chairman: *Arthi Jayaraman*

09:00-09.45	**PL9**	**V.-M. Scuturici** INSA Lyon (FR) *Laveraging artificial intelligence for materials discovery: opportunities and challenges*
09:45-10:30	**PL10**	**P. Rinke** Technical University Münich (DE) *AI-guided optimization and characterization of lignin*
10:30-10:50	**OC8**	**A. Tchagoue**, S. Pruvost, J. Duchet-Rumeau, J.F. Gerard, V. Eglin, J.N. Petit Université Claude Bernard Lyon 1 (FR) *For polymer design: multi-score reinforcement learning for high-TG polymide discovery*
10:50-11:15	**Coffee Break**	

Session F
Chairman: *Daniel Grande*

11:15-12:00	**PL11**	**U.S. Schubert,** S. Zechel, M. Ringleb, T. Koswig, J. Kimmig, Y. Köster Friedrich Schiller University Jena (DE) *High-throughput experimentation for polymers: from quantitative structure-property relationships towards application of machine-learning*
12:00-12:20	**OC9**	**M.W. Terban,** B. Hinrichsen, S. Winkler Momentum Transfer GmbH (DE) *From molecules to morphology: high-throughput X-ray scattering for multi-length-scale characterization of polymer structures*
12:20-12:40	**OC10**	**L. Misrachi** Synboli, (FR) *Synboli: accelerating the development of high performance polymer materials through AI*
13:00-14:30	**Lunch**	
17:00	**Wine tasting hosted in Bertinoro Municipal Hall**	
20:00	**Conference Dinner @Ca' de Bè Osteria Enoteca**	

Thursday, 21 May 2026 (morning)

Session G
Chairman: *Simon Harrison*

09:00-09:45 **PL12** **K. Ferji**
University of Lorraine (FR)
Machine learning fro multiscale polymer system

09:45-10:30 **PL13** **N. Ballard**
University of the Basque Country UPV/EHU (ES)
Knowledge guided machine learning for polymer science

10:30-11:00 **Coffee Break**

11:00-11:20 **OC11** **F. Catalini**, F. Conticelli, K. Massani, M.W.J. Luiten-Olieman, E. Marcantoni, S. Gabrielli
University of Camerino (IT)
Development of nanofiltration hybrid membranes for sustainable heterogeneous catalysis in continuous-flow

11:20-11:40 **OC12** **E. Ricci**, E.J. Husom
University of Edinburgh (UK)
Screening polymers for gas separations with a hybrid physics-based and data-driven strategy

11:40-12:00 **Prizes Awarding & Final Remarks**

13:15 **Shuttle Departure for Bologna Airport and Bologna Railway Station**

POSTER SESSION

Tuesday, 19 May 2026

P1 **V. Baddam**, A.Tirkkonen, R. Delannoy, J. Vaari, V. Modi, O. Pakarinen, E. Karjalainen, A.Paajanen, M.J. Jenkins
VTT Technical Research Centre of Finald Ltd (FI)
Computational prediction of glass transition in biosynthesized polyhydroxyalkanoates

P2 **S. Das,** YM. Salzano de Luna
University of Naples "Federico II" (IT)
Effect of intermolecular forces on the design of composites for pollutant removal from water: correlating an experimental and machine learning approach

P3 **E. Diomar**, T. Vidil, S. Harrisson
University of Bordeaux (FR)
Synthesis of photo-polymerizable and self-foamable oligo-hydroxyurethanes for the accelerated discovery and optimization of sustainale foams

P4 **C. Gabiron**, M. Schmitt, F. Morlet-Savary, J. Lalevée
University of Haute-Alsace (FR)
Overcoming oxygen inhibition in free radical polymerization through IPN formulation design: a design of experiments approach

P5 **J.F. Gerard**, S. Pruvost
Université de Lyon/INSA Lyon (FR)
Amethyst project 'accelerated discovery of polymers using high-throughput and artificial intelligence tools

P6 T.-E. Shui**, H. Huang**
Chinese Academy of Science (CN)
Directed assembly of large-sized gold nanoparticles by block copolymers: fabrication and photothermal properties

P7 T. Vidil, C. Le Coz, E. Grau, H. Cramail, D. Taton, S. Harrisson, **Q.C. Le Minh**, H.Mutlu, F. Bally Le Gall, K. Mougin, J. Oliveira, V. Roucoules, A. Spangenberg, T. Roland, P. Kekicheff, M. Bouquet, W. Drenckhan-Andreatta, C. Gauthier, M. Golabi, M. Essaid, L. Idoumghar, R. De Guio, H. Chibane
Institut de Science des Matériaux de Mulhouse (FR)
Accelerated discovery and optimization of high-performance green foams with controlled hierarchical architecture by light-driven processes

P8 L. Zhang**, H. Li**
Chinese Academy of Sciences (CN)
Machine learning prediction of mechanical properties of polyolefins

P9 **Y. Lin**, H. Fang, Z. Su
Changchun Institute of Applied Chemistry (CN)
Single-particle analysis of microplastics and nanoplastics using AFM-IR spectroscopy

P10 **I. Murataj**, C. Magosso, M. Perego, G. Seguini, D.J. Audus, G. Milano, F. Ferrarese Lupi
INRiM (IT)
Standardized database for data-driven design of BCP-based physical unclonable funtions

P11 **K. Pramod**, A.R.A Palmans
Eindhoven University of Technology (NL)
Targeted bio-orthogonal catalysis using transition-metal-based polymeric nanoparticels in 3D cell environments

P12 **H. Singh**, A.R.A. Palmans
Eindhoven University of Technology (NL)
Hight throughput PET-RAFT polymerization for controlling protein-polymer interactions

P13 **P. P. Singh**, G. Milano, M. Salzano De Luna
Università degli Studi di Napoli "Federico" (IT)
Machine learning prediction of physicochemical properties and adsorption performance in chitosan-based hydrogels

P14 **I Šoljić Jerbić**, J. Barbarić, B. Krneta, M. Mihaljević, A. Ljubić, M. Durrigl, M. Lac, S. Pavković
Pliva Hrvatska d.o.o, Research and Development (HR)
Design of biodegradable injectable polymer systems for local and sustained drug delivery

P15 **J. Steele**, H.A. Karimi-Varzaneh, P. Carbone
The University of Manchester (UK)
A high-throughput screening of the composition effects on thermodynamic and structural properties in styrene-butadiene rubber compounds

P16 **K. Taipe**, L. Chiaravallotti, S. Peignier, Z. Smida, S. Livi, P. Da Silva
University of Lyon – INSA Lyon (FR)
Application of machine learning in QSAR modeling to predict the repellent activity of essential oil compounds

P17 **M.W. Terban**, B. Hinrichsen, S. Winkler
Momentum Transfer GmbH (DE)
A high-throughput X-ray scattering setup for multi-length-scale characterization of polymer structures: technical capabilities

P18 **A. Thattaruthodikayil**, M. Salzano De Luna
Università di Napoli "Fedrico II" (IT)
MOF-Chitosan hybrid hydrogels and aerogels for tunable adsorption and transport in water remediation

Designing New Polymers by Combining High-Throughput and Artificial Intelligence Tool

With a worldwide production of nearly 450 million tons per year, polymer materials play a central role in our modern society. They are used in the manufacture of innumerable daily-life products, or as more sophisticated compounds in medicine, diagnostics, and fine chemistry. However, economical and new societal constraints require a more rational design and alternative synthesis, formulation and processing methods for polymer manufacturing to meet the need for greater sustainability, more virtuous end-of-life management, while maintaining optimal performances in application. Polymer-based materials of the future will be one of the pillars of the circular economy. Thus, the discovery of new polymers will lead to a paradigm shift and new methodologies for the design, processing and analysis of polymer-based materials. The recent development of high-throughput (HTP) and artificial intelligence (AI) methods has opened up enormous opportunities to tackle these challenges. While such methods are emerging in chemistry, they have not yet been implemented in Polymer Science.

Thus, the EUPOC2026 proposes the state of art in the fields related to :

1. High-throughput methods for synthesis and characterization from macromolecular architectures to physical properties, i.e. considering molecular, macromolecular, and materials scales. Inputs of polymer modelling
2. Data management using Artificial Intelligence tools from the data collection, analyses (deep learning, neuronal networks, data mining) to the specific issues related to polymers, i.e. polymer fingerprint/digital standard
3. Combination of HTP approaches with AI tools in order to take profit of machine-learning approaches for designing optimized materials.

List of topics to be addressed:

- Last developments of high-throughput methods for polymer synthesis (synthesis in flux, production of gradient-based polymer materials, X-Y generation, etc)
- Last devenopments of high-throughput methods for polymer characterization: NMR, IR, Raman, SEC, scattering methods including Tg determination, mechanical properties, gas barrier, etc
- Data collection and management such as data mining basics.
- Artificial Intelligence tools for polymer scientists. Basis on machine-learning methods – Basis on neuronal networks, deep learning, etc.
- Last developments of AI methods to polymer discovery (polymers, composites, processing)
- Last developments of combining AI tools and high-throughput methods for polymers or related materials
- How to train polymer scientists to AI tools ?
- (Flash/short) presentations for HT and AI tools suppliers