

# Meeting of the WP on crystallization of the EFCE

18/09/2024

Torino and on-line meeting

# Agenda

- Composition of the WP: new members!
- Report on the summer school 2024
- Next school (2025 or 2026?)
- Next spotlight talk spring 2025
- Planning of the next ISIC 2026 Budapest
- Any other business

# Composition of the WP

France	Delegate	Prof. Béatrice Biscans	<a href="mailto:marjatta.touh-kuitanen@aalto.fi">E-mail: marjatta.touh-kuitanen@aalto.fi</a> Université de Toulouse, CNRS-Laboratoire de Génie Chimique UMR 5503, 4 Allée Emile Monso, BP 84234, 31432 Toulouse- Cedex 4, France Tel: +33 5 34 32 36 38 E-mail: <a href="mailto:beatrice.biscans@ensiacet.fr">beatrice.biscans@ensiacet.fr</a>
	Delegate	Dr. Laurent Cassayre	Laboratoire de Génie Chimique 4, allée Emile Monso 31432 Toulouse E-mail: <a href="mailto:laurent.cassayre@toulouse.inp.fr">laurent.cassayre@toulouse.inp.fr</a>
	Delegate	Dr. Philippe Carvin	Research & Innovation, Pro Senior Principal Scientist, & 69190 SAINT-FONS – Franc E-mail: <a href="mailto:philippe.carvin@sy">philippe.carvin@sy</a>



**Laurent Cassayre** · 2nd

Research Scientist CNRS chez Laboratoire de Génie Chimique  
Toulouse / Chemical Engineering Research Center of Toulouse

# Report on the Summer school 2024

- Thanks to Ashwin Rajagopalan, Thomas Vetter, Simon Schiele and Mei Lee for the organization!

# Report on the Summer school 2024



**E  
F  
C  
E**

**Summer School on  
Crystallization**

Sign up Now!  


Seminars on Fundamentals and Applications

 **June 26<sup>th</sup> – 28<sup>th</sup> 2024**

 **Hosted by GSK in Stevenage (UK)**

 **For early Career Professionals from  
Academia (250 £) and Industry (500 £)**

 **Dr. Kevin Back, Prof. Heiko Briesen, Dr. Nick Henley, Dr. Mei Lee, Prof.  
Daniele Marchisio, Prof. Wim Noorduyn, Dr. Ashwin Rajagopalan, Prof.  
Gabriele Sadowski, Leif-Thore Deck, Dr. Kerstin Wohlgemuth**

  
As of 22 May 2024

# Report on the Summer school 2024



**E**  
**F**  
**C**  
**E**



As of 22 May 2024

## Speaker Spot-Light

Sign up Now!



**Dr. Kevin Back** wrote his PhD thesis on crystal growth and impurities in pharmaceutical crystallization. He worked on pharmaceutical crystallization for more than 15 years for AstraZeneca and Pfizer and is now Product Manager at the Cambridge Crystallographic Data Centre.

**Leif-Thore Deck** is about to finish his PhD on Crystal Nucleation Theory at ETH Zürich. He will head to the UK to continue his career as a Postdoctoral Fellow at Cambridge University.

**Prof. Heiko Briesen** holds the chair for process systems engineering at the Technical University of Munich. His work concerns the importance of crystal size and shape. He researches population balance modeling techniques and experimental crystal size and shape characterization.

**Prof. Wim Noorduin** is a professor and group leader at the Institute for Atomic and Molecular Physics in Amsterdam. His group works with self-organizing matter, specifically the interplay of crystallization and chemical reactions.

**Prof. Gabriele Sadowski** is the Director of the Laboratory for Thermodynamics at TU Dortmund University. Her work concerns complex solid-liquid equilibria in multi-component systems. She is well known for the Perturbed Chain SAFT (PC-SAFT) model.

# Report on the Summer school 2024



As of 22 May 2024

## Speaker Spot-Light

Sign up Now!



**Prof. Daniele Marchisio** is a full Professor at Politecnico di Torino. His interest lies in modeling techniques like Computational Fluid Dynamics, Molecular Dynamics, and Population Balance Modeling and their coupling in Multiscale Modelling approaches.


**Dr. Kerstin Wohlgemuth** is leading the group *crystallization and product design* at the laboratory of plant and process design at TU Dortmund University. She designs with her group innovative crystallization apparatuses and integrates them into process chains.

**Dr. Ashwin Kumar Rajagopalan** holds a PhD in chemical engineering for his work on crystal size and shape analysis at ETH Zurich. He is now a lecturer and lead investigator at the Purification and Separation Technology laboratory at the University of Manchester.

**Dr. Mei Lee** has been working on crystallization since the early 90s, first as a PhD student at Curtin University in Australia, then worked for Sanofi, and now at GSK as a scientific leader for crystallization. Her work deals with pre-Phase one all the way to commercial development.

**Dr. Nick Henley** is an Associate Director in Materials Science at GSK and has been working on salt and polymorph selection, crystallization process development and scale up with focus on earlier phase development since 2004.

# Report on the Summer school 2024



## Summer School on Crystallization Program

Sign up Now!



**Wednesday, 26 June (Starts 9am)**  
Crystal forms and thermal characterization  
Nucleation  
Populations  
Growth  
Social Activity & Dinner\*

**Thursday, 27 June**  
Thermodynamics  
Breakage & Agglomeration  
Crystallization equipment  
Process design and modeling  
Industrial case studies  
Dinner\*

**Friday, 28 June (Ends 12:30pm)**  
Collaborative work on case studies  
Wrap up

Dr. Kevin Back  
Leif-Thore Deck  
Prof. Heiko Briesen  
Prof. Wim Noorduin

Prof. Gabriele Sadowski  
Prof. Daniele Marchisio  
Dr. Kerstin Wohlgemuth  
Dr. Ashwin Rajagopalan  
Dr. Lee & Dr. Henley

\*Dinner not included

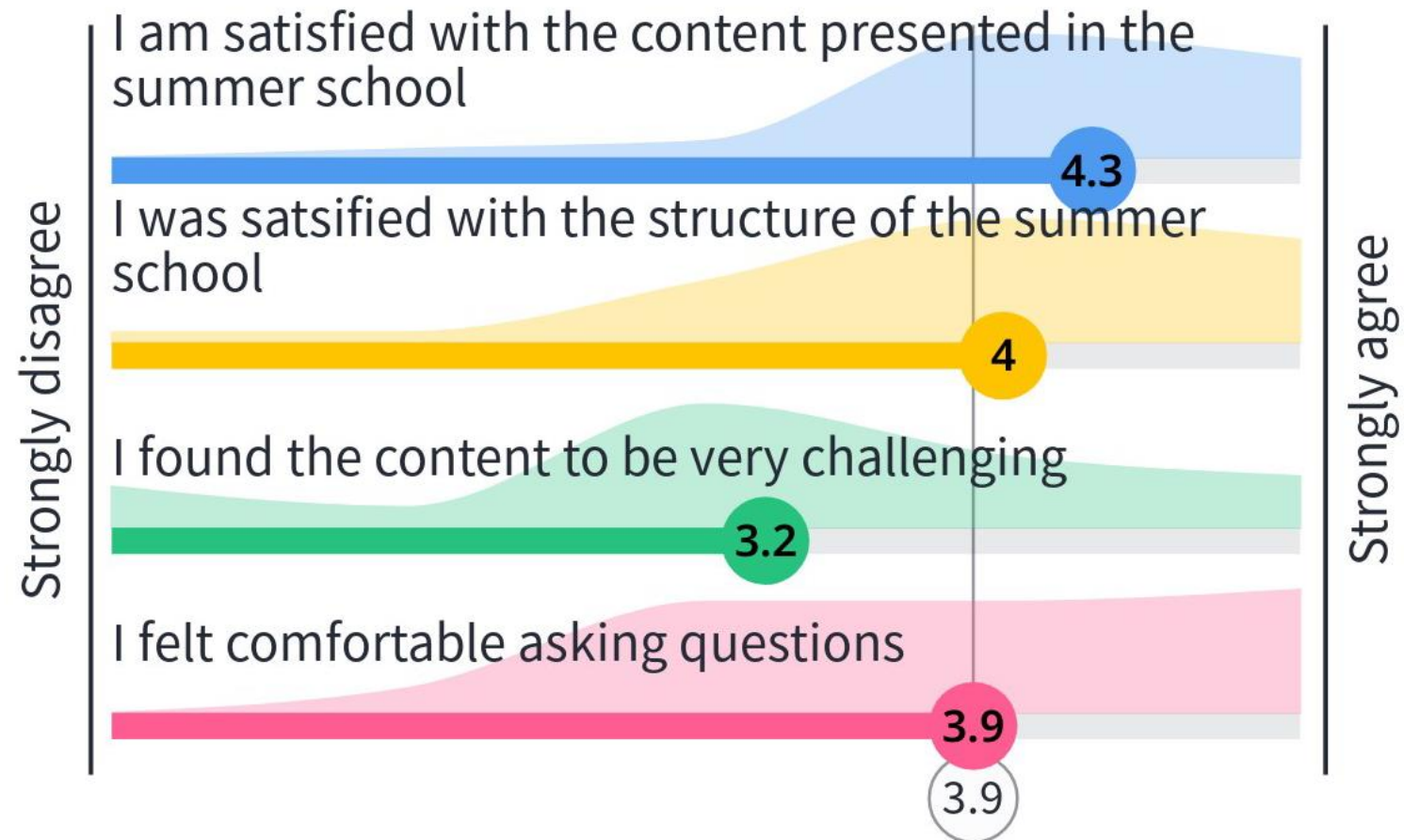


# Report on the Summer school 2024



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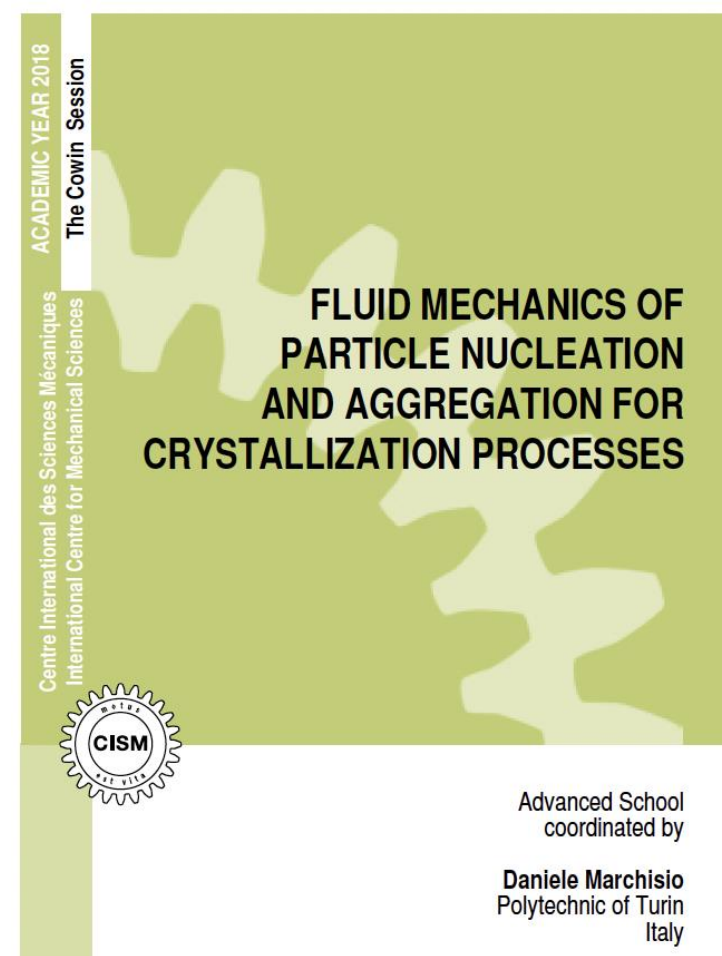
## Rate the following:





# Next school?

- The schools were not run on a regular basis
- We had one in Udine (organized by DM) in 2018
- We were supposed to have one on 2020 (cancelled)
- We had another one in June 2022 hosted by Kerstin in TU/Dortmund
- This one in Stevenage June 2024
- What about the next one?
- 2025? 2026? If 2026 together with ISIC in Budapest?

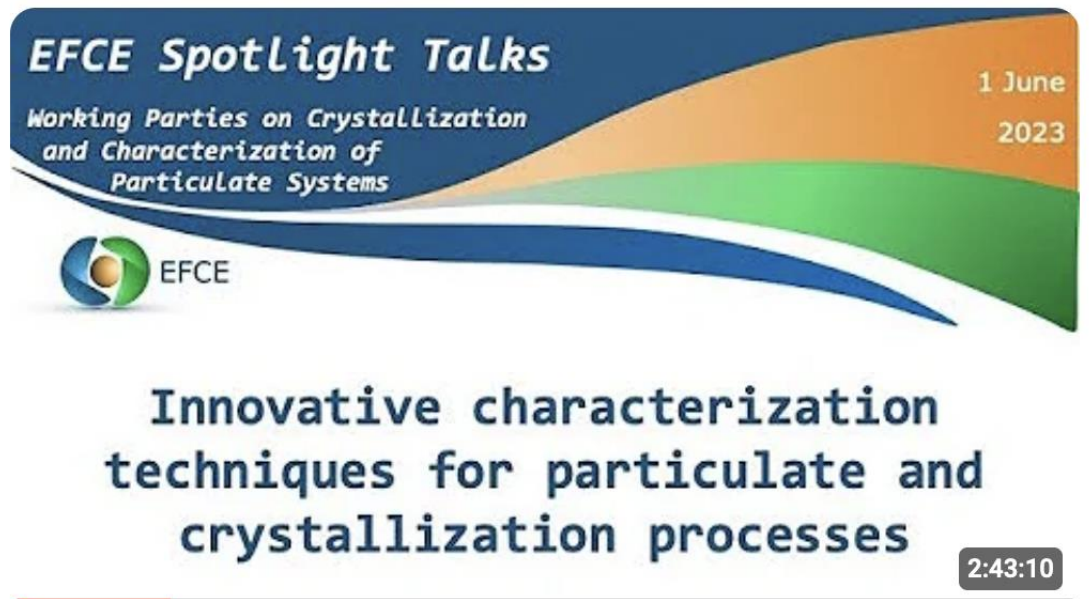
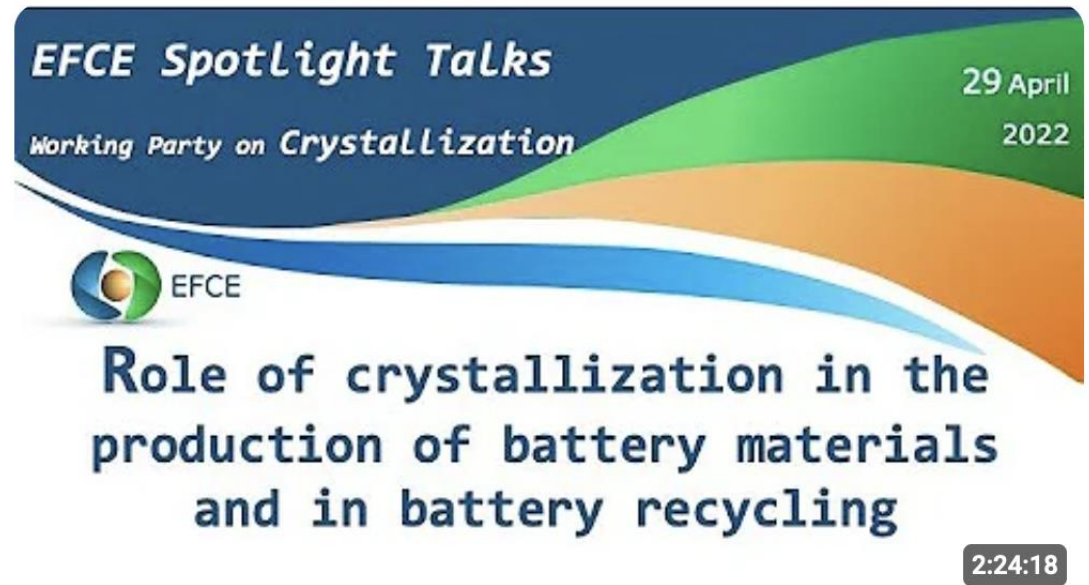


# EFCE spotlight talks



## Machine Learning and Artificial Intelligence Applications in Industrial Crystallization

1:59:22



		Regis	part	Ratio (%)
March 2024	THERMODYNAMICS AND TRANSPORT PROPERTIES	364	171	47
	MEMBRANE ENGINEERING	151	68	45
	EDUCATION	245	104	42
	STATIC ELECTRICITY IN INDUSTRY	106	52	49
	DRYING	180	87	48
	FLUID SEP	295	150	51
	LOSS PREVENTION AND SAFETY	238	112	47
	CRYSTALLIZATION	341	128	38
	CHEM REAC. ENG + PROCESS INTEN.	477	218	46
	FLUID SEP	263	118	45
FOOD	91	30	33	
May 2023	QUALITY by DESIGN	108	39	36
	MULTIPHASE FLUID FLOW	142	68	48
	HIGH PRESSURE TECH.	161	66	41
	CHEM ENG as APPLIED to MEDICINE	91	29	32
	STATIC ELECTRICITY IN INDUSTRY	46	14	30
	EARLY CAREER CHEM ENG	99	32	32
	CRYSTALLIZATION + CHARACTERIZATION PART. SYS	182	77	42
	THERMODYNAMICS AND TRANSPORT PROPERTIES	154	64	42
May 2022	DRYING	144	60	42
	MULTIPHASE FLUID FLOW	213	104	49
	MEMBRANE ENGINEERING	160	69	43
	EDUCATION	162	71	44
	MIXING	160	76	48
	CAPE	155	61	39
	HIGH PRESSURE TECH.	202	83	41
	CRYSTALLIZATION	249	113	45

EFCE spotlight talks

Next one in spring 2025?  
On what topic?

# ARTIFICIAL INTELLIGENCE in CHEMICAL ENGINEERING

13 December 2024  
Paris - France

Artificial Intelligence and Machine Learning have had in the recent past a tremendous impact on chemical engineering. On the long run they can radically change the way in which we perform research on chemical processes, we design, scale-up and optimize chemical reactors and pieces of equipment and they can potentially introduce new paradigms on chemical process control and operation.

Many are the challenges ahead for our community that can be addressed by the EFCE and its Working Parties and Sections. These can a successful journey only if the European Chemical Engineering community, both academic and industrial, is fully engaged.

In this meeting we will bring together some visionary speakers to set out the potential and the challenges. There will be the opportunity to discuss the fundamentals of artificial intelligence, deep learning and machine learning, as well as their applications to process modelling, control and the building of digital twins.

## LISTEN & INTERACT

Listen to the invited speakers and interact in discussions related the artificial intelligence and chemical engineering

## TAKING PART IN THE ROUND-TABLE

Share your point of view  
*What are the industrialists expectations on AI?  
How could academia help develop in this direction?  
What should be taught at academia?*

## CONTACT ORGANIZER

Martine.Poux@toulouse-inp.fr

## EASY ACCESS LOCATION

Hôtel MERCURE Montparnasse  
40 rue du Commandant Mouchotte  
75014 PARIS - France  
Metro 4, 6, 12, 13 - Stop : Montparnasse-Bienvenue

Registration fees: 160 €  
Registration fees (SFGP members): 120 €  
Lunch and breaks included

## REGISTER on line

# ARTIFICIAL INTELLIGENCE in CHEMICAL ENGINEERING

13 December 2024  
Paris - France

Preliminary program  
8:45 am  
5:00 pm

- ▶ **Transforming process engineering with generative artificial Intelligence**
- ▶ **AI & ML in the process industry: where we are and where we are going**
- ▶ **Different ways in which AI can be used within the organization to optimize industrial processes**
- ▶ **AI tools for process modeling and simulation: a critical overview on potentialities and limitations so far**
- ▶ **Process flowsheet generation by AI: motivation & current state**
- ▶ **Using machine learning for online 3D characterization of crystals in suspension**
- ▶ **Predicting solubility limits with machine learning**
- ▶ **Deep-learning methods for the image-based assessment of the physical stability of formulated liquids of industrial interest**

## Artur Schweidtmann

Delft University of Technology,  
The Netherlands

## Mattia Vallerio

Syensqo, Milano, Italy

## Mathieu Cura

Optimistik, Chambéry, France

## Alessandro di Pretoro

ENSIACET/Laboratoire de Génie  
Chimique, Toulouse, France

## Thibaut Neveux

EDF Lab, Chatou, France

## Anna Jaeggi

ETH Zurich, Switzerland

## Florence Vermeire

KU Leuven, Belgium

## Massimiliano Villone

Maurizio De Micco  
University of Naples Federico II, Italy

## Round table

What are the industrialists expectations on AI and how could academia help develop in this direction?

What should be taught at academia?

Registration fees: 160 €  
Registration fees (SFGP members): 120 €  
Lunch and breaks included  
[Click here to register](#)

## REGISTER on line



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75014 PARIS - France  
Metro 4, 6, 12, 13 - Stop : Montparnasse-Bienvenue

## EASY ACCESS LOCATION





# Next ISIC 2026 Budapest

- Event taking place in summer 2026
- Program defined in April-May 2026
- Review of the abstracts February-March 2026
- Deadline for abstract submission January 2026
- 2<sup>nd</sup> call for abstracts: November 2025
- 1<sup>st</sup> call for abstracts: September 2025
- Plenary speakers identified September 2025
- Announcement summer 2025

Any other business (?)