ISIC 22 / BACG 52 - Programme for Parallel Sessions

Wednesday 6th September

| Parallel Session | n A - 11.20-12.40 | | | | |
|------------------|---|--------------------|---|-------------|--|
| Session A1 | Crystallization fundamentals 1 - Auditorium B&C | | | | |
| A1.1 | Rapid, automated measurement of dynamic size distributions and size-dependent growth rates of crystal ensembles within microfluidic flow cells | Ariel Yi Hui Chua | National University of Singapore | Singapore | |
| A1.2 | Capturing interface induced concentration enhancement in situ via surface plasmon resonance spectroscopy | Ruairidh Mackay | University Of Strathclyde | UK | |
| A1.3 | Triggering the Growth of Magnesium Hydroxide Crystals in Stirred Tank Crystallizers using Sodium Hydroxide Solutions | Salvatore Romano | Università Degli Studi Di Palermo | Italy | |
| A1.4 | Facet Crystal Growth Rate Measurements of Beta-Form L-Glutamic Acid for Growth Kinetics Determination with Machine Learning | Chen Jiang | University Of Leeds | UK | |
| Session A2 | A2 Advances in industrial crystallization processes 1 - Auditorium A | | | | |
| A2.1 | Kinetic Impurity Rejection and Form Control for GDC-4379 Drug Substance via Continuous Crystallization | Andreas Stumpf | Genentech | USA | |
| A2.2 | Process Control and Design of the Continuous Crystallization of a Polymorphic Agrochemical | Montgomery Smith | Purdue University, Davidson School of Chemical Engineering | USA | |
| A2.3 | Continuous Crystallization of Monoclonal Antibodies | Torsten Stelzer | University of Puerto Rico | Puerto Rico | |
| A2.4 | Characterization of a Novel 7-Stage Continuous Crystallizer Cascade with Diaphragm-Driven Slurry Transfer | Giovanni Aprile | Technical University Of Denmark | Denmark | |
| Session A3 | iession A3 Sustainable crystallization technologies 1 - Level 1 Auditorium | | | | |
| A3.1 | Crystallisation in flow environments: smooth cooling gradients to in situ XRD analysis, a KRAICing series of crystallisers | Karen Robertson | University of Nottingham | UK | |
| A3.2 | Mechanism and kinetics of salt recoveries by seeding membrane distillation crystallization | Stefanie Flatscher | Johannes Kepler University Linz, Institute of Process Engineering | Austria | |
| A3.3 | Effects of operating parameters on crystal properties of CaCO3 during an integrated CO2 capture and mineralization process | Dharmjeet Madhav | KU Leuven, Belgium | Belgium | |
| A3.4 | Highly-efficient production of desired solid forms of drugs with improved mechanical properties via an organic solvent-free sublimation process | Xin Su | Tianjin University | China | |

| Parallel Session B - 14.40-16.00 | | | | | |
|----------------------------------|--|-------------------|-----------------------------------|--------------|--|
| Session B1 | Crystallization fundamentals 2 - Auditorium B&C | | | | |
| B1.1 | The Effect of Recirculation Rate on the Crystallization of REE Recovered using Antisolvent Crystallization in a Fluidised Bed Reactor | Jacolien Sussens | University Of Cape Town | South Africa | |
| B1.2 | Secondary Nucleation Scale-Up for Stirred Vessels | Gina Kaysan | Karlsruhe Institute of Technology | Germany | |
| B1.3 | The Scaling Up of Batch Crystallisation Processes: Small Changes, Big Impacts | Amy Robertson | AstraZeneca | UK | |
| B1.4 | Dynamic interplay of crystal growth, abrasion and shape in crystallization processes: modelling and experimental approaches | Simon Schiele | Technical University of Munich | Germany | |
| Session B2 | B2 Process modelling, design & control & digital design 1 - Auditorium A | | | | |
| B2.1 | Digital design framework for pharmaceutical crystallization processes – A case study for continuous cooling crystallization of Diphenhydramine hydrochloride | Yash Barhate | Purdue University | USA | |
| B2.2 | Evaluation of Methods for Particle Characterisation from In-Situ Sensors | Christopher Boyle | University Of Strathclyde | UK | |
| B2.3 | Model Predictive Control of Supersaturation and Crystal Size During Batch Cooling Crystallisation of Hexamine from Ethanol Solution | Tariq Mahmud | University of Leeds | UK | |
| B2.4 | Application of Deep Learning to Support Industrial Crystallization Process Development | Akeem Olaleye | APC Ltd | Ireland | |
| Session B3 | New materials & products 1 - Level 1 Auditorium | | | | |
| B3.1 | New Salts and Cocrystals of Pymetrozine with Improvements on Solubility and Humidity Stability: Experimental and Theoretical Study | Di Wu | Tianjin University | China | |
| B3.2 | Levofloxacin and Quercetin drug-GRAS co-crystal: solid-state characterization, solubility and dissolution rate investigation of a novel biologically-active system | Cecilia Fiore | Politecnico Di Torino | Italy | |
| | Novel series of Ivosidenib-Polymer cocrystals | Adam Patterson | Veranova | UK | |
| B3.4 | Co-crystal screening of novel solid forms and determination of the relationship between crystal structure and particle properties | Emmanuele Parisi | Politecnico Di Torino | Italy | |

| Parallel Session | Parallel Session C - 16.25-17.25 | | | | |
|------------------|--|-----------------|--|-------------|--|
| Session C1 | Crystallization fundamentals 3 - Auditorium B&C | | | | |
| C1.1 | Taking Cues from Elementary Chemical Kinetics: Absolute Rate Theory of Homogeneous Crystal Nucleation from Solution | Sven Schroeder | University of Leeds | UK | |
| C1.2 | Classical and non-classical nucleation mechanisms of insulin crystals | Joana Ferreira | University Of Porto | Portugal | |
| C1.3 | On the kinetics of stochastic ice nucleation from aqueous solutions | Leif-Thore Deck | Eth Zürich | Switzerland | |
| C1.4 | Prediction of API solubility: an overview of the recent developments of the SAFT-gamma Mie approach | Thomas Bernet | Imperial College London | UK | |
| Session C2 | C2 Advances in industrial crystallization processes 2 - Auditorium A | | | | |
| C2.1 | Heterogeneous crystallization on the surface of formulation additive | Hajnalka Pataki | Budapest University Of Technology And Economics | Hungary | |
| C2.2 | Deracemization of Conglomerates via Temperature Cycling and Cooling | Mercedeh Sadat | | | |
| C2.2 | | Hosseinalipour | ETH Zurich | Switzerland | |
| C2.3 | Towards protein crystallization as a tool for bio-separation: study of insulin crystallization in a meso OFR-SPC | Filipa Castro | Lepabe-feup | Portugal | |
| C2.4 | How polymer templates influence the crystallisation rate of pharmaceutical materials | Grahame Woollam | Novartis | Switzerland | |
| Session C3 | Process modelling, design & control & digital design 2 - Level 1 Auditorium | | | | |
| C3.1 | Integrated Filtration and Washing modelling of Active Pharmaceutical Ingredients and Impurities | Bhavik Mehta | Siemens Process Systems Engineering Ltd | Germany | |
| C3.2 | Temperature correction of spectra to achieve isothermal local model performance for monitoring and control of cooling crystallisation | Magdalene Chong | University Of Strathclyde | UK | |
| C3.3 | A Computationally Efficient Framework for Solving Population Balances in Crystallization Using Adaptive High-resolution Finite Volume Method | Yung-Shun Kang | Davidson School of Chemical Engineering, Purdue University | USA | |
| C3.4 | Computer aided solvent design to minimize solvent use in integrated synthesis, purification and isolation for sustainable pharmaceutical manufacturing | Chris Price | University Of Strathclyde | UK | |

Thursday 7th September

| Parallel Session | D - 11.45-13.05 | | | |
|------------------|--|-------------------------------|--|--------------|
| | Crystallization fundamentals 4 - Auditorium B&C | | | |
| D1.1 | Mesoscale clusters in the crystallization of amino acids | Michele Chen | ETH Zürich | Switzerland |
| D1.2 | Tackling Intermolecular Interactions and Transient Liquid Phases in Protein Crystallization using Molecular Rotors | Yevgeniya Karibjanova | Laboratory Of Chemical Engineering Of Toulouse | France |
| D1.3 | Modular microfluidic platform for solubility measurement, nucleation statistics and polymorph screening of active pharmaceutical ingredients. | Romain Grossier | CNRS - CINaM | France |
| D1.4 | Heterogeneous nucleation of urea from aqueous solution: a combined experimental and simulation approach | Samira Anker | University Of Strathclyde | UK |
| Session D2 | New materials & products 2 - Auditorium A | | • | |
| D2.1 | Green Synthesis of Magnolol Multicomponent Crystals for Improved Natural Antibiotics and Customizable Release Profiles | Haibin Qu | Tianjin University | China |
| D2.2 | Understanding the crystallization of complex mixtures of triglycerides: towards rational design of confectionary products with improved sustainability | Elena Simone | Polito | Italy |
| D2.3 | Separation Strategies for Tailored Molecular Weight Fractionation: The Inherent Complexity of Lignins Polydispersity During Fractional Precipitation | Arulselvan Ponnudurai | Max Planck Institute for Dynamics of Complex Technical Systems | Germany |
| D2.4 | Impact of additive concentration on stabilization and carrier particle mediated isolation of dalcetrapib nanoparticles | Peuli Ghosh | University of Limerick | Ireland |
| | Advances in industrial crystallization processes 3 - Level 1 Auditorium | | | |
| D3.1 | Crystallization of Ni-Co-Mn-Li in Battery Recycling Applications | Evangelos Stamatiou | Hatch | Canada |
| D3.2 | Controlling reaction equilibrium and crystal formation using membrane-assisted antisolvent crystallization | Sara Chergaoui | Université catholique de Louvain | Belgium |
| D3.3 | Understanding washing behavior and optimizing its efficiency during continuous particle isolation in a modular Vacuum Screw Filter (CVSF) | Justin Simons | Tu Dortmund University | Germany |
| D3.4 | Design and Characterization of Electrochemical pH-shift Crystallization Processes | Christian Kocks | Fluid Process Engineering - AVT.FVT | Germany |
| | | | | |
| Parallel Session | | | | |
| | Crystallization fundamentals 5 - Auditorium B&C | In the state of | Tony | True |
| E1.1 | How do you select a form for progression from a complex landscape? | Aneesa Al-Ani Rohan Parmer | GSK | UK |
| E1.2 E1.3 | Studying Ultra-Small Silver Nanoparticle Formation by Coupling Ultra-Fast Mixing and in-situ UV-Vis and SAXS Crystal or Amorphous? Impact of Chemical and Crystal Structure on Formation Rate | Colin Seaton | Laboratoire de Génie Chimique University Of Bradford | France UK |
| E1.4 | Crystal of Annophious impact to Chemical and Crystal structure on Pormation Rate [dentification and characterisation of mesoscale clusters in ethanolic solutions of flufenamic acid | | SSPC, University Of Limerick | |
| | Process modelling, design & control & digital design 3 - Auditorium A | Harsh Barua | 33FC, Offiversity Of Efficiency | Ireland |
| E2.1 | Deep-learning based in-situ image monitoring crystal polymorph and size distribution: modeling and validation | Zhenguo Gao | Tianjin University | China |
| E2.2 | Using a morphological population balance to develop a model-driven QBD approach for crystallisation processes | Eftychios Hadjittofis | UCB Pharma | Ireland |
| E2.3 | Two Dimensional Population Balance Model of a Cooling Crystallization Process for Particle Morphology Control | Niall Mitchell | Siemens Process Systems Engineering Ltd. | UK |
| E2.4 | Impact of a multistage cyclic crystallization process on the size and shape of plate-like crystals | Daniel Biri | Eth Zürich | Switzerland |
| | Sustainable crystallization technologies 2 - Level 1 Auditorium | Darner Sin | EU EU IU | SWILLERIANG |
| E3.1 | Recovery of metals from Lithium-ion battery recycling through simultaneous precipitation of hydroxide metal salts | Andressa Mazur | KTH | Sweden |
| E3.2 | Purification of High-Value Natural Substances from Complex Multicomponent Extracts - Towards an efficient and more sustainable process | Steffi Wünsche | Max Planck Institute For Dynamics Of Complex Technical Systems | Germany |
| E3.3 | Recovery of Spent Lithium-Ion Batteries Using a Novel Reactive Crystallization Process | Mriganka Mondal | University College Dublin | Ireland |
| E3.4 | Continuous precipitation of terephthalic acid in a back-to-monomer recycling process for PET | Clemens Mueller | Technische Universität Braunschweig | Germany |
| | | • | | _ |
| Parallel Session | F - 16.50-17.50 | | | |
| Session F1 | Crystallization Fundamentals 6: John Sherwood Session - Auditorium B&C | | | |
| F1.1 | "The Big Man" The Early Career of Professor John Sherwood (1955-1985) together with some Reflections upon his Wider Community Impact | Kevin Roberts | University of Leeds | UK |
| F1.2 | Remembering Prof John Sherwood | Rile Ristic | University of Sheffield | UK |
| F1.3 | John Sherwood: Continuity and change across the turn of the century | Ranko Vrjeli | Cranfield University | UK |
| Session F2 | New materials & products 3 - Auditorium A | | | |
| F2.1 | Piezoelectric Biomolecules for Lead-Free, Reliable, Eco-Friendly Electronics | Sarah Guerin | University of Limerick | Ireland |
| F2.2 | Crystal Structure and Solid-State Behavior of Derivatives of Praziquantel | Clément Pinètre | Sms Lab, Univ Normandie | France |
| F2.3 | Mechanical Motion and Modulation of Thermal-Actuation Properties in a Robust Organic Molecular Crystal Actuator | Jiawei Lin | Tianjin University | China |
| Session F3 | Process modelling, design & control & digital design 4 - Level 1 Auditorium | | | |
| F3.1 | Maximizing similarity: using correlation coefficients to calibrate kinetic parameters in PBMs | Álmos Orosz | Budapest University Of Technology And Economics | Hungary |
| F3.2 | Machine Learning Nucleation Collective Variables using Graph Neural Networks | Florian Markus Dietrich | University College London | UK |
| F3.3 | Machine learning for multivariate parameter identification of first-principle model: the Mg(OH)2 test case | Antonello Raponi | Politecnico di Torino | Italy |

Friday 8th September

| Parallel Session G - 10.55-12.15 | | | | |
|----------------------------------|--|-----------------------|--|--------------|
| Session G1 | Crystallization fundamentals 7 - Auditorium B&C | | | |
| G1.1 | Using sub-millisecond microfluidic mixers coupled to time-resolved in-situ photonics to study ultra-fast gold nanoparticles formation kinetics | Isaac Rodriguez Ruiz | LGC - CNRS | France |
| G1.2 | Filler surface induced heterogeneous nucleation of polymer crystals | Dominic Wadkin-snaith | The University Of Strathclyde | UK |
| G1.3 | Investigating the effect of heat exchanger roughness and surface energy on scaling during eutectic freeze crystallization. | Lerato Motsepe | University of Cape Town | South Africa |
| G1.4 | Assembling of the masses: the crystallisation of larger, more flexible pharmaceuticals | Lauren Connor | Novartis | Switzerland |
| Session G2 | 2 Advances in industrial crystallization processes 4 - Auditorium A | | | |
| | | Andrew Cashmore | Massachusetts Institute Of Technology | USA |
| G2.2 | Towards autonomous continuous slug flow crystallization for small-scale applications | Kerstin Wohlgemuth | TU Dortmund University | Germany |
| G2.3 | Machine Learning-Derived Correlations for Scale-Up and Technology Transfer of Primary Nucleation Kinetics | Cameron Brown | University of Strathclyde | UK |
| G2.4 | Automated In-line Sampling and Analysis of Crystal Slurries in Industrial Processes | Markus Honkanen | Pixact Ltd | Finland |
| Session G3 | Process modelling, design & control & digital design 5 - Level 1 Auditorium | | | |
| G3.1 | Systematic design and optimization of multistage antisolvent continuous crystallization processes | Wei Li | Loughborough University | UK |
| G3.2 | Correlating Particle Informatics with Surface Wetting Measurements | Alexandru Moldovan | Cambridge Crystallographic Data Centre | UK |
| | Systematic Framework for Model-Based Digital Design of Polymorphic Crystallization | Ilke Akturk | Purdue University | USA |
| G3.4 | Computer-Aided Solvent Section for Designing API Crystallizations to be Nucleation or Crystal Growth Dominant | Jacek Zeglinski | APC Ltd. | Ireland |