



# DECHEMA

Gesellschaft für Chemische Technik  
und Biotechnologie e.V.

## PROGRAMME

30 August – 2 September 2021 · Online Event

# ISIC 21

## 21<sup>st</sup> International Symposium on Industrial Crystallization

[www.dechema.de/ISIC\\_2021](http://www.dechema.de/ISIC_2021)



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*crystals*

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Monday, 30 August 2021

|              | Tutorial A  | Tutorial B   |                          |
|--------------|---|--|--------------------------|
| 9:00-12:30   | Industrial Crystallization Fundamentals<br>J. ter Horst/F | Industrial Aspects of Crystallization<br>M. Stepanski/CH |                          |
|              | Virtual Room 1  |  |                          |
|              | Welcome and Opening                                       |  |                          |
| 13:00        | WELCOME & OPENING REMARKS                                 |  |                          |
| <i>Chair</i> | <i>H. Lorenz/D</i>  |  |                          |
| 13:10        | PLENARY OPENING LECTURE<br>J.M. Garcia Ruiz/E             |  |                          |
| 13:50        | KEYNOTE LECTURE<br>J. ter Horst/F                         |  |                          |
| 14:15        | Discussion with speakers                                  |  |                          |
| 14:30        | Coffee Break  |  |                          |
|              | Virtual Room 1  | Virtual Room 2   | Virtual Room 3           |
|              | Kinetics I  | Separation of Enantiomers I                              | Integrated Processes I   |
| <i>Chair</i> | <i>A. Myerson/USA</i>                                     | <i>G. Coquerel/F</i>                                     | <i>E. Verdurand/CH</i>   |
| 14:45        | S. Kulkarni/USA   | F. Breviglieri/CH  | J. von Langermann/D      |
| 15:05        | L. Bosetti/CH   | C. Xiouras/B   | F. Destro/I              |
| 15:25        | S. Schiele/D  | M. Charpentier/UK  | M. Bäumlér/D             |
| 15:45        | R. Miller/UK  | S. Bhandari/D  | Discussion with speakers |
| 16:05        | Discussion with speakers                                  | Discussion with speakers                                 |                          |
| 16:25        | Opening Poster Discussion / Session I                     |  |                          |
| 17:30        | Social Get-together: Quiz                                 |  |                          |

Time: UTC +2

Tuesday, 31 August 2021

|              | Virtual Room 1                                   | Virtual Room 2                      | Virtual Room 3                    |
|--------------|--|-------------------------------------|-----------------------------------|
|              | <b>Process Monitoring</b>                        | <b>Separation of Enantiomers II</b> | <b>Industrial Applications I</b>  |
| <i>Chair</i> | <i>M. Louhi-Kultanen/FIN</i>                     | <i>M. Mazzotti/CH</i>               | <i>P. Carvin/F</i>                |
| 8:30         | J. Lins/D  | B. Bodák/CH                         | A. Zwijnenburg/NL                 |
| 8:50         | T. Kathyola/UK                                   | K. Funakoshi/J                      | J. Gebauer/D                      |
| 9:10         | D. Wirz/D  | J. Sun/CN                           | A. Collas/B                       |
| 9:30         | A. Jaeggi/CH                                     | F. Cascella/D                       | I. Østergaard/DK                  |
| 9:50         | Discussion with speakers                         | Discussion with speakers            | Discussion with speakers          |
| 10:10        | Coffee Break                                     |                                     |                                   |
| 10:30        | Poster Session II                                |                                     |                                   |
| 12:00        | Lunch Break                                      |                                     |                                   |
|              | Virtual Room 1                                   |                                     |                                   |
|              | Plenary and Keynote Lectures                     |                                     |                                   |
| <i>Chair</i> | <i>R. Geertman/B</i>                             |                                     |                                   |
| 12:45        | <b>PLENARY LECTURE</b><br>C. Melches/D           |                                     |                                   |
| <i>Chair</i> | <i>A. Zwijnenburg/NL</i>                         |                                     |                                   |
| 13:25        | <b>KEYNOTE LECTURE</b><br>E. Rigaut/CH           |                                     |                                   |
| 13:50        | <b>KEYNOTE LECTURE</b><br>A. Chow/SGP            |                                     |                                   |
| 14:15        | Discussion with speakers                         |                                     |                                   |
| 14:30        | Coffee Break                                     |                                     |                                   |
|              | Virtual Room 1                                   | Virtual Room 2                      | Virtual Room 3                    |
|              | <b>Kinetics II</b>                               | <b>Continuous Crystallization</b>   | <b>Industrial Applications II</b> |
| <i>Chair</i> | <i>P. Daudey/NL</i>                              | <i>Z. Nagy/UK &amp; USA</i>         | <i>M. Lee/UK</i>                  |
| 14:50        | G. Kaysan/D                                      | N. Rey/CH                           | C. Burcham/USA                    |
| 15:10        | A. Cashmore/UK                                   | K. Tacsí/H                          | H. Yao/USA                        |
| 15:30        | D. Guse/D  | J. Gänsch/D                         | T. Rosenbaum/USA                  |
| 15:50        | Discussion with speakers                         | Discussion with speakers            | Discussion with speakers          |
| 16:05        | Short Break                                      |                                     |                                   |
|              | Virtual Room 1                                   |                                     |                                   |
|              | Plenary Lecture                                  |                                     |                                   |
| <i>Chair</i> | <i>A. Seidel-Morgenstern/D</i>                   |                                     |                                   |
| 16:15        | <b>PLENARY LECTURE</b><br>R. Braatz/USA          |                                     |                                   |
| 17:00        | End of second day                                |                                     |                                   |
|              | WP Meeting in the evening (invited participants) |                                     |                                   |

Wednesday, 1 September 2021

|              | Virtual Room 1                            | Virtual Room 2                  | Virtual Room 3                         |
|--------------|---|---------------------------------|--|
|              | <b>Modeling</b>                           | <b>Reactive Crystallization</b> | <b>Contributions to Sustainability</b> |
| <i>Chair</i> | <i>D. Marchisio/I</i>                     | <i>B. Biscans/F</i>             | <i>A. Lewis/ZA</i>                     |
| 8:30         | J. Unno/J                                 | J. Gómez-Morales/E              | F. Vassallo/I                          |
| 8:50         | V. Tenberg/D                              | H. Takiyama/J                   | L. Motsepe/ZA                          |
| 9:10         | C. Ma/UK                                  | C. Ruiz Vasquez/F               | M. Rodriguez Pascual/NL                |
| 9:30         | M. Ukrainczyk/IRL                         | L. Metzger/D                    | R. Halfwerk/NL                         |
| 9:50         | Discussion with speakers                  | Discussion with speakers        | Discussion with speakers               |
| 10:10        | Coffee Break                              |                                 |  |
| 10:30        | Poster Session III                        |                                 |  |
| 12:00        | Lunch Break                               |                                 |  |
|              | Plenary and Keynote Lectures              |                                 |  |
| <i>Chair</i> | <i>C. Melches/D</i>                       |                                 |  |
| 12:45        | <b>PLENARY LECTURE</b><br>B. Biscans/F    |                                 |  |
| <i>Chair</i> | <i>M. Stepanski/CH</i>                    |                                 |  |
| 13:25        | <b>KEYNOTE LECTURE</b><br>D. Marchisio/I  |                                 |  |
| 13:50        | <b>KEYNOTE LECTURE</b><br>R. Rousseau/USA |                                 |  |
| 14:15        | Discussion with speakers                  |                                 |  |
| 14:30        | Coffee Break                              |                                 |  |
|              | Virtual Room 1                            | Virtual Room 2                  | Virtual Room 3                         |
|              | <b>Crystalline Phase Behaviour</b>        | <b>Battery Materials</b>        | <b>Integrated Processes II</b>         |
| <i>Chair</i> | <i>J. Gomez Morales/E</i>                 | <i>M. Rauls/D</i>               | <i>B. Glennon/IRL</i>                  |
| 14:50        | Y. Liu/CN                                 | M. Para/I                       | C. Steenweg/D                          |
| 15:10        | R. Mani/FIN                               | R. Berk/D                       | W. Wu/USA                              |
| 15:30        | F. Marques Penha/S                        | M. Le Page Mostefa/F            | N. Mitchell/UK                         |
| 15:50        | Discussion with speakers                  | Discussion with speakers        | Discussion with speakers               |
| 16:05        | Short Break                               |                                 |  |
|              | Plenary Lecture                           |                                 |  |
| <i>Chair</i> | <i>M. Rauls/D</i>                         |                                 |  |
| 16:15        | <b>PLENARY LECTURE</b><br>D. Green/USA    |                                 |  |
| 17:00        | End of third day                          |                                 |  |

Thursday, 2 September 2021

|              | Virtual Room 1  | Virtual Room 2   | Virtual Room 3           |
|--------------|---|--|--------------------------|
|              | Microfluidic Techniques                                     | Lectures to Honor Gerda v. Rosmalen & Special Techniques | Special Techniques       |
| <i>Chair</i> | <i>K. Wohlgemuth/D</i>                                      | <i>J. ter Horst/F &amp; D. Wei/CN</i>                    | <i>A. Chow/SGP</i>       |
| 8:30         | F. Ibis/NL  | A. Lewis/ZA  | S. Shikha/SGP            |
| 8:50         | G. Peybernes/F  | B. Eral/NL   | W. Tian/UK               |
| 9:10         | R. Cedeno/F   | K. Tanaka/J  | J. Wang/CN               |
| 9:30         | A. Nelson/SGP   | N. Ramos/D   | S. Kwon/HK               |
| 9:50         | Discussion with speakers                                    | Discussion with speakers                                 | Discussion with speakers |
| 10:10        | Coffee Break  |  |                          |
| 10:30        | Poster Session IV   |  |                          |
| 11:30        | Lunch Break   |  |                          |
|              | Plenary and Keynote Lectures                                |  |                          |
| <i>Chair</i> | <i>H. Lorenz/D</i>  |  |                          |
| 12:15        | PLENARY LECTURE<br>H. Cölfen/D                              |  |                          |
| 12:55        | KEYNOTE LECTURE<br>A. Pallipurath/UK                        |  |                          |
| 13:20        | EFCE PRIZE AWARD LECTURE 2020 / 2021<br>A.K. Rajagopalan/CH |  |                          |
| 13:45        | Discussion with speakers                                    |  |                          |
| 14:00        | Closing & Announcement of ISIC 22                           |  |                          |
| 14:15        | End of lecture programme                                    |  |                          |
| 14:30        | Tutorial C  |  |                          |
|              | Modeling, Monitoring & Control<br>Z. Nagy/UK & USA          |  |                          |
| 17:30        | End of the conference                                       |  |                          |

## Monday, 30 August 2021

09:00 – 12:30

## TUTORIAL A

**Industrial Crystallization Fundamentals**

J. ter Horst<sup>1</sup>, E. Vlieg<sup>2</sup>; A. Flood<sup>3</sup>; <sup>1</sup> Université de Rouen Normandie, Mont-Saint-Aignan/F; <sup>2</sup> University of Nijmegen/NL; <sup>3</sup> Vidyasirimedhi Institute of Science and Technology (VISTEC), Wangchan, Rayong/TH

09:00 – 12:30

## TUTORIAL B

**Industrial Aspects of Crystallization**

M. Stepanski<sup>1</sup>; E. Verdurand<sup>2</sup>; C. Pudack<sup>3</sup>; E. Temmel<sup>1</sup>; <sup>1</sup> Sulzer Chemtech Ltd., Winterthur/CH; <sup>2</sup> DSM Nutritional Products AG, Sisseln/CH; <sup>3</sup> KBR Plinke GmbH/D

## Monday, 30 August 2021

## Welcome and Opening

Virtual Room 1

13:00 **WELCOME & OPENING**

*Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D*

13:10

**PLENARY OPENING LECTURE****Wonderful crystal patterns in nature**

J.M. Garcia Ruiz<sup>1</sup>; <sup>1</sup> CSIC-University of Granada/E

13:50

**KEYNOTE LECTURE****An Industrial Toolbox for Resolution & Deracemization of Chiral Compounds through Crystallization**

J. ter Horst<sup>1</sup>; <sup>1</sup> Université de Rouen Normandie, Mont-Saint-Aignan/F

14:15

**Discussion with speakers**

14:30

## Coffee Break

## Kinetics I

Virtual Room 1

*Chair: A. Myerson, Massachusetts Institute of Technology, Cambridge/USA*

14:45

**A combined modeling and experimental approach to study the nucleation kinetics**

S. Kulkarni<sup>1</sup>; G. Wood<sup>1</sup>; E. Santiso<sup>2</sup>; C. Liu<sup>2</sup>; F. Cao<sup>3</sup>; <sup>1</sup> Pfizer Inc. Worldwide Research and Development, Groton/USA; <sup>2</sup> North Carolina State University, Raleigh, North Carolina/USA; <sup>3</sup> Pfizer Inc. Worldwide Research and Development, La Jolla/USA

15:05

**Surface secondary nucleation: the role of thermodynamics**

L. Bosetti<sup>1</sup>; B. Ahn<sup>1</sup>; M. Mazzotti<sup>1</sup>; <sup>1</sup> ETH Zurich/CH

15:25

**3D imaging yields a physical explanation for growth rate dispersion and size dependent growth**

S. Schiele<sup>1</sup>; R. Hupfer<sup>1</sup>; H. Briesen<sup>1</sup>; <sup>1</sup> TU München, Freising/D

15:45

**Modelling diffusive mixing in antisolvent crystallisation**

R. Miller<sup>1</sup>; J. Sefcik<sup>1</sup>; L. Lue<sup>2</sup>; <sup>1</sup> University of Strathclyde/ CMAC, Glasgow/UK; <sup>2</sup> University of Strathclyde, Glasgow/UK

16:05

**Discussion with speakers**

16:25

## Opening Poster Discussions / Poster Session I

17:30

**Social Get-together: Quiz**

## Monday, 30 August 2021

09:00 – 12:30

## TUTORIAL A

**Industrial Crystallization Fundamentals**

J. ter Horst<sup>1</sup>, E. Vlieg<sup>2</sup>; A. Flood<sup>3</sup>; <sup>1</sup> Université de Rouen Normandie, Mont-Saint-Aignan/F; <sup>2</sup> University of Nijmegen/NL; <sup>3</sup> Vidyasirimedhi Institute of Science and Technology (VISTEC), Wangchan, Rayong/TH

09:00 – 12:30

## TUTORIAL B

**Industrial Aspects of Crystallization**

M. Stepanski<sup>1</sup>; E. Verdurand<sup>2</sup>; C. Pudack<sup>3</sup>; E. Temmel<sup>1</sup>; <sup>1</sup> Sulzer Chemtech Ltd., Winterthur/CH; <sup>2</sup> DSM Nutritional Products AG, Sisseln/CH; <sup>3</sup> KBR Plinke GmbH/D

## Monday, 30 August 2021

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J.M. Garcia Ruiz<sup>1</sup>; <sup>1</sup> CSIC-University of Granada/E

13:50

**KEYNOTE LECTURE****An Industrial Toolbox for Resolution & Deracemization of Chiral Compounds through Crystallization**

J. ter Horst<sup>1</sup>; <sup>1</sup> Université de Rouen Normandie, Mont-Saint-Aignan/F

14:15

**Discussion with speakers**

14:30

Coffee Break

## Separation of Enantiomers I

Virtual Room 2

*Chair: G. Coquerel, Université de Rouen/F*

14:45

**Improving the understanding of deracemisation via temperature cycles for enhanced process design and implementation**

F. Breveglieri<sup>1</sup>; B. Bodák<sup>1</sup>; M. Mazzotti<sup>1</sup>; <sup>1</sup> ETH Zurich/CH

15:05

**Development of continuous crystallization-enhanced deracemization processes with PAT monitoring**

C. Xiouras<sup>1</sup>; F. Cameli<sup>2</sup>; G. Belletti<sup>3</sup>; R. Venkatraman<sup>4</sup>; H. Meekes<sup>3</sup>; E. Vlieg<sup>3</sup>; G. Stefanidis<sup>2</sup>; J. ter Horst<sup>4</sup>; <sup>1</sup> Janssen Research & Development, Beerse/B; <sup>2</sup> University of Leuven/B; <sup>3</sup> Radboud University, Nijmegen/NL; <sup>4</sup> University of Strathclyde, Glasgow/UK

15:25

**Co-crystal screening: methods to optimize success rate**

M. Charpentier<sup>1</sup>; J. Devogelaer<sup>2</sup>; H. Meekes<sup>2</sup>; R. de Gelder<sup>2</sup>; E. Vlieg<sup>2</sup>; K. Johnston<sup>1</sup>; J. ter Horst<sup>1</sup>; <sup>1</sup> University of Strathclyde, Glasgow/UK; <sup>2</sup> Radboud University, Nijmegen/NL

15:45

**A Shortcut Model to Evaluate Continuous Preferential Crystallization for Conglomerates Forming Systems**

S. Bhandari<sup>1</sup>; H. Lorenz<sup>2</sup>; A. Seidel-Morgenstern<sup>2</sup>; <sup>1</sup> Otto von Guericke University Magdeburg/D; <sup>2</sup> Max Planck Institut für Dynamik komplexer technischer Systeme / Otto-von-Guericke University Magdeburg/D

16:05

**Discussion with speakers**

16:25

**Opening Poster Discussions / Poster Session I**

17:30

**Social Get-together: Quiz**

## Monday, 30 August 2021

09:00 – 12:30

## TUTORIAL A

**Industrial Crystallization Fundamentals**

J. ter Horst<sup>1</sup>, E. Vlieg<sup>2</sup>; A. Flood<sup>3</sup>; <sup>1</sup> Université de Rouen Normandie, Mont-Saint-Aignan/F; <sup>2</sup> University of Nijmegen/NL; <sup>3</sup> Vidyasirimedhi Institute of Science and Technology (VISTEC), Wangchan, Rayong/TH

09:00 – 12:30

## TUTORIAL B

**Industrial Aspects of Crystallization**

M. Stepanski<sup>1</sup>; E. Verdurand<sup>2</sup>; C. Pudack<sup>3</sup>; E. Temmel<sup>1</sup>; <sup>1</sup> Sulzer Chemtech Ltd., Winterthur/CH; <sup>2</sup> DSM Nutritional Products AG, Sisseln/CH; <sup>3</sup> KBR Plinke GmbH/D

## Monday, 30 August 2021

## Welcome and Opening

Virtual Room 1

13:00 **WELCOME & OPENING**

*Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D*

13:10

**PLENARY OPENING LECTURE****Wonderful crystal patterns in nature**

J.M. Garcia Ruiz<sup>1</sup>; <sup>1</sup> CSIC-University of Granada/E

13:50

**KEYNOTE LECTURE****An Industrial Toolbox for Resolution & Deracemization of Chiral Compounds through Crystallization**

J. ter Horst<sup>1</sup>; <sup>1</sup> Université de Rouen Normandie, Mont-Saint-Aignan/F

14:15

**Discussion with speakers**

14:30

## Coffee Break

## Integrated Processes I

Virtual Room 3

*Chair: E. Verdurand, DSM Nutrition Products, Sisseln/CH*

14:45

**Integrated application and scale-up of a selective crystallization in an enzyme-catalysed synthesis process**

J. Neuburger<sup>1</sup>; D. Hülsewede<sup>1</sup>; F. Belov<sup>1</sup>; P. Süß<sup>2</sup>; U. Menyess<sup>2</sup>; J. von Langermann<sup>1</sup>; <sup>1</sup> University of Rostock/D; <sup>2</sup> Enzymicals AG, Greifswald/D

15:05

**A model-based framework for design and control of integrated crystallization, filtration and drying of active pharmaceutical ingredients**

F. Destro<sup>1</sup>; M. Barolo<sup>1</sup>; Z. Nagy<sup>2</sup>; <sup>1</sup> University of Padova/I; <sup>2</sup> Purdue University, West Lafayette/USA

15:25

**Upscaling the production of a novel, high potential phosphate binding nanomaterial**

M. Bäuml<sup>1</sup>; S. Schwaminger<sup>1</sup>; D. von der Haar-Leistl<sup>2</sup>; S. Berensmeier<sup>1</sup>; <sup>1</sup> Technical University of Munich, Garching/D; <sup>2</sup> Fraunhofer IVV, Freising/D

15:45

**Discussion with speakers**

16:00

## End of session

16:25

**Opening Poster Discussions / Poster Session I**

17:30

**Social Get-together: Quiz**



## Tuesday, 31 August 2021

| Process Monitoring   |  | Virtual Room 1 |
|--|--|----------------|
| <i>Chair: M. Louhi-Kultanen, Aalto University, Espoo/FIN</i>   |  |                |
| 08:30  | <b>Imaging techniques to understand and characterize agglomeration during batch cooling crystallization</b><br>J. Lins <sup>1</sup> ; U. Ebeling <sup>1</sup> ; H. Ramezani <sup>1</sup> ; K. Wohlgenuth <sup>1</sup> ; <sup>1</sup> TU Dortmund University, Dortmund/D  |                |
| 08:50  | <b>Probing the Structural Evolution of a Molecular Solute in Solution with Advanced X-ray Analytical Techniques: A Study of Imidazole Crystallization</b><br>L. Al-Madhagi <sup>1</sup> ; B. Evans <sup>1</sup> ; T. Kathyola <sup>1</sup> ; E. Willneff <sup>1</sup> ; S. Schroeder <sup>1</sup> ; <sup>1</sup> University of Leeds/UK  |                |
| 09:10  | <b>Image-based inline measurement of crystal size distributions</b><br>D. Wirz <sup>1</sup> ; A. Seidel-Morgenstern <sup>2</sup> ; M. Hofmann <sup>1</sup> ; E. Temmel <sup>3</sup> ; H. Lorenz <sup>4</sup> ; H. Bart <sup>1</sup> ; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D; <sup>3</sup> Sulzer Chemtech Ltd, Allschwil/CH; <sup>4</sup> Max Planck Institute for Dynamics Complex Technical Systems, Magdeburg/D |                |
| 09:30  | <b>Multidimensional Characterization of Platelets in Particulate Suspensions via Machine Learning</b><br>A. Jaeggi <sup>1</sup> ; A. Rajagopalan <sup>1</sup> ; M. Morari <sup>2</sup> ; M. Mazzotti <sup>1</sup> ; <sup>1</sup> ETH Zurich/CH; <sup>2</sup> University of Pennsylvania, Philadelphia/USA  |                |
| 09:50  | Discussion with speakers   |                |
| 10:10  | Coffee Break   |                |
| 10:30  | Poster Session II  |                |
| 12:00  | Lunch Break  |                |
| Plenary and Keynote Lectures   |  | Virtual Room 1 |
| <i>Chair: R. Geertman, Janssen R&amp;D BE, Beerse/B</i>  |  |                |
| 12:45  | <b>PLENARY LECTURE</b><br><b>Developments in large scale industrial crystallization</b><br>C. Melches <sup>1</sup> ; <sup>1</sup> GEA Messo GmbH, Duisburg/D   |                |
| <i>Chair: A. Zwijnenburg, Nouryon Industrial Chemicals - Salt, Deventer/NL</i>   |  |                |
| 13:25  | <b>KEYNOTE LECTURE</b><br><b>An empirical modelling approach of layer crystallization supercharging strategies</b><br>E. Rigaut <sup>1</sup> ; E. Temmel <sup>2</sup> ; M. Stepanski <sup>1</sup> ; <sup>1</sup> Sulzer Chemtech, Winterthur/CH; <sup>2</sup> Sulzer Chemtech, Allschwil/CH  |                |
| 13:50  | <b>KEYNOTE LECTURE</b><br><b>Pharmaceutical cocrystals: from screening to process development and pre-formulation</b><br>A. Chow <sup>1</sup> ; <sup>1</sup> Agency for Science, Technology & Research (A*STAR), Singapore/SGP   |                |
| 14:15  | Discussion with speakers   |                |
| 14:30  | Coffee Break   |                |
| Kinetics II  |  | Virtual Room 1 |
| <i>Chair: P. Daudey, TU Delft/NL</i>   |  |                |
| 14:50  | <b>Possibilities and limitations of secondary contact nucleation of subcooled melt emulsions: A microfluidic approach</b><br>G. Kaysan <sup>1</sup> ; M. Kind <sup>1</sup> ; <sup>1</sup> Karlsruhe Institute of Technology (KIT), Karlsruhe/D   |                |
| 15:10  | <b>Secondary Nucleation and Crystal Growth in the Metastable Zone</b><br>A. Cashmore <sup>1</sup> ; M. Haw <sup>2</sup> ; M. Lee <sup>3</sup> ; J. Sefcik <sup>1</sup> ; <sup>1</sup> University of Strathclyde, CMAC Future Manufacturing Research Hub, Glasgow/UK; <sup>2</sup> University of Strathclyde, Glasgow/UK; <sup>3</sup> GlaxoSmithKline, Stevenage/UK  |                |
| 15:30  | <b>Experimental determination of solids formation times in the coprecipitation of Cu/Zn based catalyst precursors and their significance for catalyst preparation</b><br>D. Guse <sup>1</sup> ; S. Polierer <sup>1</sup> ; S. Wild <sup>1</sup> ; K. Herrera Delgado <sup>1</sup> ; S. Pitter <sup>1</sup> ; M. Kind <sup>1</sup> ; <sup>1</sup> Karlsruhe Institute of Technology (KIT), Karlsruhe/D  |                |
| 15:50  | Discussion with speakers   |                |
| 16:05  | Short Break  |                |
| Plenary Lecture  |  | Virtual Room 1 |
| <i>Chair: A. Seidel-Morgenstern, Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg &amp; Otto von Guericke University Magdeburg/D</i> |  |                |
| 16:15  | <b>PLENARY LECTURE</b><br><b>Modeling, sensing, design and control of crystallizing proteins</b><br>R. Braatz <sup>1</sup> ; <sup>1</sup> Massachusetts Institute of Technology, Cambridge/USA   |                |
| 17:00  | End of second day  |                |

## Tuesday, 31 August 2021

| Separation of Enantiomers II   |  | Virtual Room 2 |
|--|--|----------------|
| <i>Chair: M. Mazzotti, ETH Zürich/CH</i>   |  |                |
| 08:30  | <b>Modeling crystallization-based deracemization techniques: guidelines for selecting a favorable process for production</b><br>B. Bodák <sup>1</sup> ; M. Mazzotti <sup>1</sup> ; <sup>1</sup> ETH Zürich/CH  |                |
| 08:50  | <b>Preferential Crystallization of Glutamic Acid Associated by Polymorphism</b><br>K. Funakoshi <sup>1</sup> ; S. Naito <sup>1</sup> ; K. Hayashi <sup>1</sup> ; <sup>1</sup> National Institute of Technology, Suzuka College, Suzuka/J   |                |
| 09:10  | <b>Additive-assisted Preferential Crystallization of Racemic Component: A Case of Norvaline</b><br>J. Sun <sup>1</sup> ; Y. Wang <sup>1</sup> ; Z. Gao <sup>1</sup> ; W. Tang <sup>1</sup> ; J. Gong <sup>1</sup> ; <sup>1</sup> Tiangjin University, Tianjin/CN   |                |
| 09:30  | <b>Preferential Crystallization of the API Guaifenesin in a fluidized bed crystallizer: Seeding strategy development</b><br>F. Cascella <sup>1</sup> ; J. Gänsch <sup>2</sup> ; A. Seidel-Morgenstern <sup>1</sup> ; H. Lorenz <sup>2</sup> ; <sup>1</sup> Max-Planck-Institut für Dynamik komplexer technischer Systeme & Otto-von-Guericke-Universität, Magdeburg/D; <sup>2</sup> Max Planck Institut für Dynamik komplexer technischer Systeme, Magdeburg/D |                |
| 09:50  | <b>Discussion with speakers</b>  |                |
| 10:10  | <b>Coffee Break</b>  |                |
| 10:30  | <b>Poster Session II</b>   |                |
| 12:00  | <b>Lunch Break</b>   |                |
| Plenary and Keynote Lectures   |  | Virtual Room 1 |
| <i>Chair: R. Geertman, Janssen R&amp;D BE, Beerse/B</i>  |  |                |
| 12:45  | <b>PLENARY LECTURE</b><br><b>Developments in large scale industrial crystallization</b><br>C. Melches <sup>1</sup> ; <sup>1</sup> GEA Messo GmbH, Duisburg/D   |                |
| <i>Chair: A. Zwijnenburg, Nouryon Industrial Chemicals - Salt, Deventer/NL</i>   |  |                |
| 13:25  | <b>KEYNOTE LECTURE</b><br><b>An empirical modelling approach of layer crystallization supercharging strategies</b><br>E. Rigaut <sup>1</sup> ; E. Temmel <sup>2</sup> ; M. Stepanski <sup>1</sup> ; <sup>1</sup> Sulzer Chemtech, Winterthur/CH; <sup>2</sup> Sulzer Chemtech, Allschwil/CH  |                |
| 13:50  | <b>KEYNOTE LECTURE</b><br><b>Pharmaceutical cocrystals: from screening to process development and pre-formulation</b><br>A. Chow <sup>1</sup> ; <sup>1</sup> Agency for Science, Technology & Research (A*STAR), Singapore/SGP   |                |
| 14:15  | <b>Discussion with speakers</b>  |                |
| 14:30  | <b>Coffee Break</b>  |                |
| Continuous Crystallization   |  | Virtual Room 2 |
| <i>Chair: Z. Nagy, Loughborough University/UK &amp; Purdue University/USA</i>  |  |                |
| 14:50  | <b>Development of a Continuous Crystallisation Process in a Stirred-Tank Cascade through Process Analytical Technology Sensors</b><br>N. Rey <sup>1</sup> ; P. Riedlberger <sup>1</sup> ; <sup>1</sup> Institute of Chemistry and Biotechnology, Zurich University of Applied Sciences (ZHAW), Wädenswil/CH  |                |
| 15:10  | <b>Development of continuous crystallization technologies for direct processing of a flow reaction mixture</b><br>K. Tacsí <sup>1</sup> ; Z. Nagy <sup>1</sup> ; G. Marosi <sup>1</sup> ; H. Pataki <sup>1</sup> ; <sup>1</sup> Budapest University of Technology and Economics (BME), Budapest/H  |                |
| 15:30  | <b>Continuous racemate resolution in coupled fluidized bed crystallizers: Experimental parametric study</b><br>J. Gänsch <sup>1</sup> ; E. Temmel <sup>2</sup> ; H. Lorenz <sup>1</sup> ; A. Seidel-Morgenstern <sup>3</sup> ; <sup>1</sup> Max Planck Institute for Dynamics Complex Technical Systems, Magdeburg/D; <sup>2</sup> Sulzer Chemtech Ltd, Allschwil/CH; <sup>3</sup> Otto von Guericke University, Magdeburg/D                                   |                |
| 15:50  | <b>Discussion with speakers</b>  |                |
| 16:05  | <b>Short Break</b>   |                |
| Plenary Lecture  |  | Virtual Room 1 |
| <i>Chair: A. Seidel-Morgenstern, Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg &amp; Otto von Guericke University Magdeburg/D</i> |  |                |
| 16:15  | <b>PLENARY LECTURE</b><br><b>Modeling, sensing, design and control of crystallizing proteins</b><br>R. Braatz <sup>1</sup> ; <sup>1</sup> Massachusetts Institute of Technology, Cambridge/USA   |                |
| 17:00  | <b>End of second day</b>   |                |

## Tuesday, 31 August 2021

| Industrial Applications I  |   | Virtual Room 3 |
|--|---|----------------|
| <i>Chair: P. Carvin, Solvay, Lyon/F</i>  |   |                |
| 08:30  | <b>In-line monitoring of sulphate precipitation behavior in industrial crystallizers</b><br>J. Westerink <sup>1</sup> ; W. Barnard <sup>1</sup> ; J. Pek <sup>1</sup> ; A. Soare <sup>1</sup> ; A. Schokker <sup>1</sup> ; <u>A. Zwijnenburg</u> <sup>1</sup> ; <sup>1</sup> Nouryon, Deventer/NL   |                |
| 08:50  | <b>Passive Acoustic Emission for Crystallization</b><br><u>J. Gebauer</u> <sup>1</sup> ; <sup>1</sup> Bayer AG, Leverkusen/D  |                |
| 09:10  | <b>Design, development and scale-up of a skid-based selective dissolution apparatus using liquid cyclonic classifiers and heat exchangers for tailoring crystalline product attributes and crystallization process intensification</b><br><u>A. Collas</u> <sup>1</sup> ; <sup>1</sup> Janssen Research & Development, Beerse/B   |                |
| 09:30  | <b>Polymorphic Control and Scale-up Strategies for Antisolvent Crystallization by Three Different Feedback Controls</b><br><u>I. Østergaard</u> <sup>1</sup> ; B. Szilagyi <sup>2</sup> ; Heidi Lopez de Diego <sup>3</sup> ; Zoltan K. Nagy <sup>2</sup> ; Haiyan Qu <sup>1</sup> ; <sup>1</sup> University of Southern Denmark, Odense/DK; <sup>2</sup> Purdue University, West Lafayette, Indiana/USA; <sup>3</sup> Lundbeck A/S, Copenhagen/DK                          |                |
| 09:50  | <b>Discussion with speakers</b>   |                |
| 10:10  | <b>Coffee Break</b>   |                |
| 10:30  | <b>Poster Session II</b>  |                |
| 12:00  | <b>Lunch Break</b>  |                |
| Plenary and Keynote Lectures   |   | Virtual Room 1 |
| <i>Chair: R. Geertman, Janssen R&amp;D BE, Beerse/B</i>  |   |                |
| 12:45  | <b>PLENARY LECTURE</b><br><b>Developments in large scale industrial crystallization</b><br><u>C. Melches</u> <sup>1</sup> ; <sup>1</sup> GEA Messo GmbH, Duisburg/D   |                |
| <i>Chair: A. Zwijnenburg, Nouryon Industrial Chemicals - Salt, Deventer/NL</i>   |   |                |
| 13:25  | <b>KEYNOTE LECTURE</b><br><b>An empirical modelling approach of layer crystallization supercharging strategies</b><br><u>E. Rigaut</u> <sup>1</sup> ; E. Temmel <sup>2</sup> ; M. Stepanski <sup>1</sup> ; <sup>1</sup> Sulzer Chemtech, Winterthur/CH; <sup>2</sup> Sulzer Chemtech, Allschwil/CH  |                |
| 13:50  | <b>KEYNOTE LECTURE</b><br><b>Pharmaceutical cocrystals: from screening to process development and pre-formulation</b><br><u>A. Chow</u> <sup>1</sup> ; <sup>1</sup> Agency for Science, Technology & Research (A*STAR), Singapore/SGP   |                |
| 14:15  | <b>Discussion with speakers</b>   |                |
| 14:30  | <b>Coffee Break</b>   |                |
| Industrial Applications II   |   | Virtual Room 3 |
| <i>Chair: M. Lee, GlaxoSmithKline, Stevenage, Hertfordshire/UK</i>   |   |                |
| 14:50  | <b>Development of a Continuous Crystallization with Periodic Wet Milling for Particle Size Control</b><br><u>C. Burcham</u> <sup>1</sup> ; F. Calado <sup>2</sup> ; N. Mitchell <sup>2</sup> ; S. Myers <sup>1</sup> ; V. Svoboda <sup>3</sup> ; <sup>1</sup> Eli Lilly and Company, Indianapolis/USA; <sup>2</sup> Process Systems Enterprise, London/UK; <sup>3</sup> Pfizer Inc. Worldwide Research and Development, Sandwich/UK   |                |
| 15:10  | <b>Kinetic Modelling &amp; In-Silico Parametric Analysis of Impurity Inclusion in the Crystallisation of a Pharmaceutical Molecule</b><br><u>H. Yao</u> <sup>4</sup> ; G. Taylor <sup>1</sup> ; B. Williams <sup>2</sup> ; N. Mitchell <sup>2</sup> ; R. Yule <sup>3</sup> ; <sup>1</sup> GSK, Stevenage/UK; <sup>2</sup> PSE - A Siemens Business, London/UK; <sup>3</sup> GSK, Upper Providence/USA; <sup>4</sup> GlaxoSmithKline, Colledgeville/USA                      |                |
| 15:30  | <b>Comparison of One Dimensional and Two Dimensional Population Balance Models of a Crystallization Process for a Needle Shaped API</b><br><u>T. Rosenbaum</u> <sup>1</sup> ; V. Mbachu <sup>1</sup> ; N. Mitchell <sup>2</sup> ; J. Gamble <sup>3</sup> ; P. Cho <sup>1</sup> ; J. Engstrom <sup>1</sup> ; <sup>1</sup> Bristol-Myers Squibb, New Brunswick/USA; <sup>2</sup> Process Systems Enterprise Limited, London/UK; <sup>3</sup> Bristol-Myers Squibb, Moreton/UK |                |
| 15:50  | <b>Discussion with speakers</b>   |                |
| 16:05  | <b>Short Break</b>  |                |
| Plenary Lecture  |   | Virtual Room 1 |
| <i>Chair: A. Seidel-Morgenstern, Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg &amp; Otto von Guericke University Magdeburg/D</i> |   |                |
| 16:15  | <b>PLENARY LECTURE</b><br><b>Modeling, sensing, design and control of crystallizing proteins</b><br><u>R. Braatz</u> <sup>1</sup> ; <sup>1</sup> Massachusetts Institute of Technology, Cambridge/USA   |                |
| 17:00  | <b>End of second day</b>  |                |

## Wednesday, 1 September 2021

|       |  | Modeling   | Virtual Room 1 |
|-------|--|--|----------------|
|       |  | <i>Chair: B.G. Lakatos, University of Veszprém/HR</i>          |                |
| 08:30 | <b>Mathematical optimization of partially seeded cooling crystallization accompanied by agglomeration and breakage of crystals</b><br>J. Unno <sup>1</sup> ; I. Hirasawa <sup>1</sup> ; <sup>1</sup> Waseda University, Tokyo/J  |  |                |
| 08:50 | <b>Separation of Solid Solutions Using Counter-Current Crystallization</b><br>V. Tenberg <sup>1</sup> ; S. Münzberg <sup>1</sup> ; M. Sadeghi <sup>1</sup> ; H. Lorenz <sup>1</sup> ; A. Seidel-Morgenstern <sup>2</sup> ; <sup>1</sup> MPI for Dynamics of Complex Technical Systems, Magdeburg/D; <sup>2</sup> Otto von Guericke University / MPI for Dynamics of Complex Technical Systems, Magdeburg/D           |  |                |
| 09:10 | <b>Morphological Population Balance Modelling of Crystallisation Processes with Heating and Cooling Cycles</b><br>C. Ma <sup>1</sup> ; A. Rizvi <sup>1</sup> ; T. Izumi <sup>2</sup> ; K. Roberts <sup>1</sup> ; <sup>1</sup> University of Leeds/UK; <sup>2</sup> Pfizer R&D UK Limited, Sandwich, Kent /UK   |  |                |
| 09:30 | <b>Streamlining an Early Phase Crystallisation Development using In-Silico Predictive Modelling and Raman Spectroscopy</b><br>M. Ukrainczyk <sup>1</sup> ; J. Zeglinski <sup>1</sup> ; B. Glennon <sup>1</sup> ; R. Vanierschot <sup>2</sup> ; A. Collas <sup>2</sup> ; <sup>1</sup> APC Ltd., Dublin/IRL; <sup>2</sup> Janssen Pharmaceuticals, Beerse/B  |  |                |
| 09:50 | <b>Discussion with speakers</b>  |  |                |
| 10:10 | <b>Coffee Break</b>  |  |                |
| 10:30 | <b>Poster Session III</b>  |  |                |
| 12:00 | <b>Lunch Break</b>   |  |                |
|       |  | Plenary and Keynote Lectures                                   | Virtual Room 1 |
|       |  | <i>Chair: C. Melches, GEA Messo GmbH, Duisburg/D</i>           |                |
| 12:45 | <b>PLENARY LECTURE</b><br><b>Recovery of critical metals from battery waste by leaching and precipitation processes</b><br>B. Biscans <sup>1</sup> ; <sup>1</sup> University of Toulouse, CNRS, INP, UPS, Toulouse/F   |  |                |
|       |  | <i>Chair: M. Stepanski, Sulzer Chemtech Ltd, Winterthur/CH</i> |                |
| 13:25 | <b>KEYNOTE LECTURE</b><br><b>Development of a Modelling Framework for the Co-Precipitation of NMC Hydroxide as Precursor for Lithium Battery Cathodes</b><br>M. Shiea <sup>1</sup> ; M. Para <sup>1</sup> ; G. Tronci <sup>1</sup> ; A. Buffo <sup>1</sup> ; G. Boccardo <sup>1</sup> ; D. Marchisio <sup>1</sup> ; <sup>1</sup> Politecnico di Torino, Turin/I  |  |                |
| 13:50 | <b>KEYNOTE LECTURE</b><br><b>Combining reaction with crystallization for process improvement and intensification in continuous manufacturing of antibiotics</b><br>H. Salami <sup>1</sup> ; M. McDonald <sup>1</sup> ; P. Harris <sup>1</sup> ; C. Lagerman <sup>1</sup> ; M. Grover <sup>1</sup> ; A. Bommarius <sup>1</sup> ; R. Rousseau <sup>1</sup> ; <sup>1</sup> Georgia Institute of Technology, Atlanta/USA |  |                |
| 14:15 | <b>Discussion with speakers</b>  |  |                |
| 14:30 | <b>Coffee Break</b>  |  |                |
|       |  | Crystalline Phase Behaviour                                    | Virtual Room 1 |
|       |  | <i>Chair: J. Gómez Morales, CSIC - University of Granada/E</i> |                |
| 14:50 | <b>A plastically bent crystal: the correlation between crystal structure and mechanical properties</b><br>Y. Liu <sup>1</sup> ; S. Wu <sup>1</sup> ; J. Gong <sup>1</sup> ; <sup>1</sup> Tianjin University, Tianjin/CN  |  |                |
| 15:10 | <b>Organic Mesocrystals: A new strategy to enhance the drug dissolution</b><br>R. Mani <sup>1</sup> ; M. Louhi-Kultanen <sup>1</sup> ; <sup>1</sup> Aalto University School of Chemical Engineering, Espoo/FIN   |  |                |
| 15:30 | <b>Can surfactant self-assemblies be used to control polymorphism?</b><br>F. Marques Penha <sup>1</sup> ; F. Ibis <sup>2</sup> ; A. Gopalan <sup>2</sup> ; J. Meijlink <sup>2</sup> ; H. Eral <sup>2</sup> ; <sup>1</sup> KTH Royal Institute of Technology, Stockholm/S; <sup>2</sup> Delft University of Technology, Delft/NL  |  |                |
| 15:50 | <b>Discussion with speakers</b>  |  |                |
| 16:05 | <b>Short Break</b>   |  |                |
|       |  | Plenary Lecture  | Virtual Room 1 |
|       |  | <i>Chair: M. Rauls, BASF SE, Ludwigshafen/D</i>                |                |
| 16:15 | <b>PLENARY LECTURE</b><br><b>Industrial crystallization – establishing solid state properties for both downstream processing and product performance (tentative title)</b><br>D. Green <sup>1</sup> ; <sup>1</sup> GlaxoSmithKline, Collegeville/USA   |  |                |
| 17:00 | <b>End of third day</b>  |  |                |

## Wednesday, 1 September 2021

| Reactive Crystallization   |   | Virtual Room 2 |
|--|---|----------------|
| <i>Chair: B. Biscans, University of Toulouse, CNRS, INP, UPS, Toulouse/F</i> |   |                |
| 08:30  | <b>Crystallization of (lanthanide, calcium) phosphate nanophosphors</b><br>J. Gómez-Morales <sup>1</sup> ; R. Fernández-Penas <sup>1</sup> ; C. Verdugo-Escamilla <sup>1</sup> ; D. Choquesillo-Lazarte <sup>1</sup> ; C. Drouet <sup>2</sup> ; F. Oltolina <sup>3</sup> ; M. Prat <sup>3</sup> ; M. Iafisco <sup>4</sup> ; J. Fernández-Sánchez <sup>5</sup> ; <sup>1</sup> Instituto Andaluz de Ciencias de la Tierra, Consejo Superior de Investigaciones Científicas, Armilla/E; <sup>2</sup> CNRS / University of Toulouse/F; <sup>3</sup> University of Piemonte Orientale, Novara/I; <sup>4</sup> CNR - National Research Council of Italy, Faenza/I; <sup>5</sup> University of Granada/E |                |
| 08:50  | <b>Control of Reaction Crystallization of Organic Compounds Considering with Supersaturation Profile</b><br>H. Takiyama <sup>1</sup> ; <sup>1</sup> Tokyo University of Agriculture and Technology, Tokyo/J   |                |
| 09:10  | <b>A compartmental-based approach for the modelling of a vortex precipitation reactor for nuclear energy applications</b><br>C. Ruiz Vasquez <sup>1</sup> ; N. Lebaz <sup>2</sup> ; D. Mangin <sup>2</sup> ; M. Bertrand <sup>3</sup> ; E. Saikali <sup>4</sup> ; M. Rodio <sup>4</sup> ; G. Bois <sup>4</sup> ; U. Bieder <sup>4</sup> ; <sup>1</sup> CEA Marcoule, Villeurbanne, France/F; <sup>2</sup> LAGEPP, Université de Lyon, CNRS UMR5007, Lyon/F; <sup>3</sup> CEA, DEN, DMRC, Université Montpellier, Marcoule/F; <sup>4</sup> CEA, DEN, STMF, Saclay/F  |                |
| 09:30  | <b>Model-based design and control of precipitation processes in industrial applications</b><br>L. Metzger <sup>1</sup> ; M. Kespe <sup>1</sup> ; T. Beierling <sup>1</sup> ; M. Voges <sup>1</sup> ; <sup>1</sup> BASF SE, Ludwigshafen/D   |                |
| 09:50  | <b>Discussion with speakers</b>   |                |
| 10:10  | <b>Coffee Break</b>   |                |
| 10:30  | <b>Poster Session III</b>   |                |
| 12:00  | <b>Lunch Break</b>  |                |
| Plenary and Keynote Lectures   |   | Virtual Room 1 |
| <i>Chair: C. Melches, GEA Messo GmbH, Duisburg/D</i>                         |   |                |
| 12:45  | <b>PLENARY LECTURE</b><br><b>Recovery of critical metals from battery waste by leaching and precipitation processes</b><br>B. Biscans <sup>1</sup> ; <sup>1</sup> University of Toulouse, CNRS, INP, UPS, Toulouse/F  |                |
| <i>Chair: M. Stepanski, Sulzer Chemtech Ltd, Winterthur/CH</i>               |   |                |
| 13:25  | <b>KEYNOTE LECTURE</b><br><b>Development of a Modelling Framework for the Co-Precipitation of NMC Hydroxide as Precursor for Lithium Battery Cathodes</b><br>M. Shiea <sup>1</sup> ; M. Para <sup>1</sup> ; G. Tronci <sup>1</sup> ; A. Buffo <sup>1</sup> ; G. Boccardo <sup>1</sup> ; D. Marchisio <sup>1</sup> ; <sup>1</sup> Politecnico di Torino, Turin/I   |                |
| 13:50  | <b>KEYNOTE LECTURE</b><br><b>Combining reaction with crystallization for process improvement and intensification in continuous manufacturing of antibiotics</b><br>H. Salami <sup>1</sup> ; M. McDonald <sup>1</sup> ; P. Harris <sup>1</sup> ; C. Lagerman <sup>1</sup> ; M. Grover <sup>1</sup> ; A. Bommarius <sup>1</sup> ; R. Rousseau <sup>1</sup> ; <sup>1</sup> Georgia Institute of Technology, Atlanta/USA  |                |
| 14:15  | <b>Discussion with speakers</b>   |                |
| 14:30  | <b>Coffee Break</b>   |                |
| Battery Materials  |   | Virtual Room 2 |
| <i>Chair: M. Rauls, BASF SE, Ludwigshafen/D</i>                              |   |                |
| 14:50  | <b>Coprecipitation of Ni<sub>x</sub>Mn<sub>y</sub>Co<sub>1-x-y</sub>(OH)<sub>2</sub> as precursor for ion lithium batteries: influence of mixing and operating conditions</b><br>M. Para <sup>1</sup> ; M. Alidoost <sup>1</sup> ; M. Shiea <sup>1</sup> ; A. Buffo <sup>1</sup> ; G. Boccardo <sup>1</sup> ; R. Pisano <sup>1</sup> ; A. Barresi <sup>1</sup> ; D. Marchisio <sup>1</sup> ; <sup>1</sup> Politecnico di Torino/I   |                |
| 15:10  | <b>Impact of Sulphate Intercalation on the Morphology of Co-Precipitated Battery Material Precursors</b><br>R. Berk <sup>1</sup> ; L. Metzger <sup>1</sup> ; T. Beierling <sup>1</sup> ; M. Rauls <sup>1</sup> ; <sup>1</sup> BASF SE Ludwigshafen/D  |                |
| 15:30  | <b>Recycling process of lithium from batteries by Li<sub>2</sub>CO<sub>3</sub> precipitation</b><br>M. Le Page Mostefa <sup>1</sup> ; C. Baumann <sup>1</sup> ; H. Muhr <sup>1</sup> ; <sup>1</sup> LRGP - UMR 7274 CNRS, Nancy/F   |                |
| 15:50  | <b>Discussion with speakers</b>   |                |
| 16:05  | <b>Short Break</b>  |                |
| Plenary Lecture  |   | Virtual Room 1 |
| <i>Chair: M. Rauls, BASF SE, Ludwigshafen/D</i>                              |   |                |
| 16:15  | <b>PLENARY LECTURE</b><br><b>Industrial crystallization – establishing solid state properties for both downstream processing and product performance (tentative title)</b><br>D. Green <sup>1</sup> ; <sup>1</sup> GlaxoSmithKline, Collegeville/USA  |                |
| 17:00  | <b>End of third day</b>   |                |

## Wednesday, 1 September 2021

| Contributions to Sustainability                                |  | Virtual Room 3 |
|--|--|----------------|
| <i>Chair: A. Lewis, University of Cape Town/ZA</i>             |  |                |
| 08:30  | <b>Selective crystallisation of magnesium and calcium hydroxides from industrial waste brines: a pilot study</b><br>F. Vassallo <sup>1</sup> ; D. La Corte <sup>1</sup> ; N. Cancilla <sup>1</sup> ; M. Bevacqua <sup>2</sup> ; A. Tamburini <sup>1</sup> ; A. Cipollina <sup>1</sup> ; G. Micale <sup>1</sup> ; <sup>1</sup> University of Palermo/I;<br><sup>2</sup> ResourSEAs Srl, Palermo/I   |                |
| 08:50  | <b>Investigating the effect of surface properties on ice scaling in Eutectic Freeze Crystallization</b><br>L. Motsepe <sup>1</sup> ; <sup>1</sup> University of Cape Town/ZA   |                |
| 09:10  | <b>Experimental review of a scraped-stirred crystallizer design for Eutectic Freeze Crystallization</b><br>M. Rodriguez Pascual <sup>1</sup> ; D. Xevgenos <sup>2</sup> ; <sup>1</sup> Water Energy Intelligence, Schiedam/NL; <sup>2</sup> TU Delft/NL  |                |
| 09:30  | <b>A sub-zero crystallization process for the recovery of lactose</b><br>R. Halfwerk <sup>1</sup> ; D. Yntema <sup>2</sup> ; J. Van Spronsen <sup>3</sup> ; A. Van der Padt <sup>4</sup> ; <sup>1</sup> Wageningen University/Wetsus European Centre of Excellence for Sustainable Water Technology, Wageningen/NL; <sup>2</sup> Wetsus European Centre of Excellence for Sustainable Water Technology, Leeuwarden/NL; <sup>3</sup> Cool Separations BV, Portugaal/NL; <sup>4</sup> FrieslandCampina/Wageningen University, Amersfoort /NL |                |
| 09:50  | <b>Discussion with speakers</b>  |                |
| 10:10  | Coffee Break   |                |
| 10:30  | Poster Session III   |                |
| 12:00  | Lunch Break  |                |
| Plenary and Keynote Lectures                                   |  | Virtual Room 1 |
| <i>Chair: C. Melches, GEA Messo GmbH, Duisburg/D</i>           |  |                |
| 12:45  | <b>PLENARY LECTURE</b><br><b>Recovery of critical metals from battery waste by leaching and precipitation processes</b><br>B. Biscans <sup>1</sup> ; <sup>1</sup> University of Toulouse, CNRS, INP, UPS, Toulouse/F   |                |
| <i>Chair: M. Stepanski, Sulzer Chemtech Ltd, Winterthur/CH</i> |  |                |
| 13:25  | <b>KEYNOTE LECTURE</b><br><b>Development of a Modelling Framework for the Co-Precipitation of NMC Hydroxide as Precursor for Lithium Battery Cathodes</b><br>M. Shiea <sup>1</sup> ; M. Para <sup>1</sup> ; G. Tronci <sup>1</sup> ; A. Buffo <sup>1</sup> ; G. Boccoardo <sup>1</sup> ; D. Marchisio <sup>1</sup> ; <sup>1</sup> Politecnico di Torino, Turin/I   |                |
| 13:50  | <b>KEYNOTE LECTURE</b><br><b>Combining reaction with crystallization for process improvement and intensification in continuous manufacturing of antibiotics</b><br>H. Salami <sup>1</sup> ; M. McDonald <sup>1</sup> ; P. Harris <sup>1</sup> ; C. Lagerman <sup>1</sup> ; M. Grover <sup>1</sup> ; A. Bommarius <sup>1</sup> ; R. Rousseau <sup>1</sup> ; <sup>1</sup> Georgia Institute of Technology, Atlanta/USA   |                |
| 14:15  | <b>Discussion with speakers</b>  |                |
| 14:30  | Coffee Break   |                |
| Integrated Processes II  |  | Virtual Room 3 |
| <i>Chair: B. Glennon, University College Dublin/IRL</i>        |  |                |
| 14:50  | <b>Integrated Process Design of Continuous Solid-Liquid Separation, Washing, and Drying for Crystal Suspensions with Varying Crystal Shapes</b><br>C. Steenweg <sup>1</sup> ; J. Habicht <sup>1</sup> ; G. Schembecker <sup>1</sup> ; K. Wohlgemuth <sup>1</sup> ; <sup>1</sup> TU Dortmund University, Dortmund/D   |                |
| 15:10  | <b>Utilization of Quality-by-Control for rapid process design of agrochemical crystallization.</b><br>W. Wu <sup>1</sup> ; C. Chappelow <sup>2</sup> ; M. Kodam <sup>3</sup> ; P. Larsen <sup>3</sup> ; P. McGough <sup>3</sup> ; J. Patton <sup>2</sup> ; A. Shinkle <sup>2</sup> ; Z. Nagy <sup>1</sup> ; <sup>1</sup> Purdue University, West Lafayette/USA; <sup>2</sup> Corteva Agriscience, Midland/USA; <sup>3</sup> Corteva Agriscience, Indianapolis/USA  |                |
| 15:30  | <b>Digital Design of crystallization process: Application of a mechanistic morphological crystallizer model to improve powder flowability via aspect ratio reduction</b><br>N. Mitchell <sup>1</sup> ; S. Douieb <sup>2</sup> ; F. Calado <sup>1</sup> ; U. Cocchini <sup>2</sup> ; P. Marzoli <sup>1</sup> ; E. Hadjittofis <sup>2</sup> ; J. Uyttersprot <sup>2</sup> ; N. Carly <sup>2</sup> ; J. Mantanus <sup>2</sup> ; <sup>1</sup> PSE - A Siemens Business, London/UK; <sup>2</sup> UCB Pharma SA, Anderlecht/B                    |                |
| 15:50  | <b>Discussion with speakers</b>  |                |
| 16:05  | Short Break  |                |
| Plenary Lecture  |  | Virtual Room 1 |
| <i>Chair: M. Rauls, BASF SE, Ludwigshafen/D</i>                |  |                |
| 16:15  | <b>PLENARY LECTURE</b><br><b>Industrial crystallization – establishing solid state properties for both downstream processing and product performance (tentative title)</b><br>D. Green <sup>1</sup> ; <sup>1</sup> GlaxoSmithKline, Collegeville/USA   |                |
| 17:00  | End of third day   |                |

## Thursday, 2 September 2021

| Microfluidic Techniques   |  | Virtual Room 1 |
|---|--|----------------|
| <i>Chair: K. Wohlgemuth, TU Dortmund/D</i>  |  |                |
| 08:30   | <b>Nucleation kinetics of Calcium Oxalate Monohydrate as a function of supersaturation and pH quantified with droplet microfluidics</b><br>F. Ibis <sup>1</sup> ; T. Wang Yu <sup>1</sup> ; F. Marques Penha <sup>1</sup> ; D. Ganguly <sup>1</sup> ; M. Alhaji Nuhu <sup>1</sup> ; A. van der Heijden <sup>1</sup> ; H. Kramer <sup>1</sup> ; H. Eral <sup>1</sup> ;<br><sup>1</sup> TU Delft/NL  |                |
| 08:50   | <b>Microfluidics platform for polymorph screening directly from powder</b><br>G. Peybernes <sup>1</sup> ; R. Grossier <sup>1</sup> ; F. Villard <sup>2</sup> ; P. Letellier <sup>2</sup> ; N. Candoni <sup>1</sup> ; S. Veessler <sup>1</sup> ; <sup>1</sup> Aix-Marseille University & CNRS, CINaM, Marseille/F; <sup>2</sup> Technologie Servier, Orléans/F  |                |
| 09:10   | <b>Nucleation in Sessile Microdroplet Arrays: Accounting for Diffusive Interactions</b><br>R. Cedeno <sup>1</sup> ; R. Grossier <sup>2</sup> ; A. Flood <sup>3</sup> ; N. Candoni <sup>4</sup> ; S. Veessler <sup>4</sup> ; <sup>1</sup> CNRS - Aix Marseille Université / Vidyasirimedhi Institute of Science and Technology (VISTEC), Marseille/F; <sup>2</sup> CNRS, Marseille/F; <sup>3</sup> Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong/T; <sup>4</sup> CNRS - Aix-Marseille University, Marseille/F |                |
| 09:30   | <b>Embedded droplet printing for pharmaceutical drug particle synthesis</b><br>A. Nelson <sup>1</sup> ; J. Xie <sup>2</sup> ; S. Khan <sup>2</sup> ; P. Doyle <sup>3</sup> ; <sup>1</sup> Singapore-MIT Alliance for Research and Technology, Singapore/SGP; <sup>2</sup> National University of Singapore, Singapore/SGP; <sup>3</sup> Massachusetts Institute of Technology; Singapore-MIT Alliance for Research and Technology, Cambridge/USA   |                |
| 09:50   | <b>Discussion with speakers</b>  |                |
| 10:10   | <b>Coffee Break</b>  |                |
| 10:30   | <b>Poster Session IV</b>   |                |
| 11:30   | <b>Lunch Break</b>   |                |
| Plenary and Keynote Lectures  |  | Virtual Room 1 |
| <i>Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems &amp; Otto von Guericke University, Magdeburg/D</i> |  |                |
| 12:15   | <b>PLENARY LECTURE</b><br><b>Nucleation theories, 80 years research on nucleation</b><br>H. Cölfen <sup>1</sup> ; <sup>1</sup> Department of Physical Chemistry, University of Konstanz/D  |                |
| 12:55   | <b>KEYNOTE LECTURE</b><br><b>Understanding the Solutions You Crystallise from: The Molecular Basis of Co-solvency and Conformational Changes by X-ray Pair Distribution Function Measurements and Modelling</b><br>A. Pallipurath <sup>1</sup> ; B. Evans <sup>2</sup> ; L. Al-Madhagi <sup>2</sup> ; A. Pugejs <sup>2</sup> ; S. Schroeder <sup>2</sup> ; <sup>1</sup> University of of Leeds/UK; <sup>2</sup> School of Chemical and Process Engineering, University of Leeds/UK   |                |
| 13:20   | <b>EFCE PRIZE AWARD LECTURE 2020 / 2021</b><br><b>A Dual Projection System to Characterize Crystallization Processes: Design and Applications</b><br>A.K. Rajagopalan, ETH Zurich/CH   |                |
| 13:45   | <b>Discussion with speakers</b>  |                |
| 14:00   | <b>Closing &amp; Announcement 22<sup>nd</sup> ISIC</b>   |                |
| 14:15   | <b>End of lecture programme</b>  |                |

## Thursday, 2 September 2021

14:30 – 17:30

## TUTORIAL C

**Modeling, Monitoring and Control of Crystallization Systems**Z.K. Nagy<sup>1</sup>; R. Braatz<sup>2</sup>; E. Simone<sup>3</sup>; N. Yazdanpanah<sup>4</sup>; B. Szilagy<sup>5</sup>; <sup>1</sup> Loughborough University, Leicestershire/UK and Purdue University/USA; <sup>2</sup> MIT, USA; <sup>3</sup> Leeds University/UK; <sup>4</sup> Procegen/USA; <sup>5</sup> Purdue University/USA

## Thursday, 2 September 2021

| Lectures to Honor Gerda v. Rosmalen & Special Techniques  |  | Virtual Room 2 |
|---|--|----------------|
| <i>Chairs: J. ter Horst, Université de Rouen Normandie, Mont-Saint-Aignan/F; D. Wei, Tianjin University of Science and Technology/PRC</i> |  |                |
| 08:30   | <b>Unique approaches to problem solving in Industrial Crystallization: Remembering Gerda van Rosmalen</b><br>A. Lewis <sup>1</sup> ; <sup>1</sup> University of Cape Town/ZA   |                |
| 08:50   | <b>Steering crystallization with light, flow and soft matter</b><br>B. Eral <sup>1</sup> ; <sup>1</sup> Delft University of Technology/NL  |                |
| 09:10   | <b>Impurities and oiling-out brought us better results</b><br>K. Tanaka <sup>1</sup> ; <sup>1</sup> CHUGAI PHARMACEUTICAL. CO., LTD., Kita-ku, Tokyo/J   |                |
| 09:30   | <b>An efficient strategy for manipulating the crystal morphology of active pharmaceutical ingredients in stirred systems</b><br>N. Ramos <sup>1</sup> ; R. Diodone <sup>2</sup> ; P. Hidber <sup>2</sup> ; M. Kind <sup>1</sup> ; <sup>1</sup> Karlsruhe Institut of Technology, Karlsruhe/D; <sup>2</sup> F. Hoffmann-La Roche AG, Basel/CH |                |
| 09:50   | <b>Discussion with speakers</b>  |                |
| 10:10   | Coffee Break   |                |
| 10:30   | <b>Poster Session IV</b>   |                |
| 11:30   | Lunch Break  |                |

| Plenary and Keynote Lectures  |   | Virtual Room 1 |
|---|---|----------------|
| <i>Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems &amp; Otto von Guericke University, Magdeburg/D</i> |   |                |
| 12:15   | <b>PLENARY LECTURE</b><br><b>Nucleation theories, 80 years research on nucleation</b><br>H. Cölfen <sup>1</sup> ; <sup>1</sup> Department of Physical Chemistry, University of Konstanz/D   |                |
| 12:55   | <b>KEYNOTE LECTURE</b><br><b>Understanding the Solutions You Crystallise from: The Molecular Basis of Co-solvency and Conformational Changes by X-ray Pair Distribution Function Measurements and Modelling</b><br>A. Pallipurath <sup>1</sup> ; B. Evans <sup>2</sup> ; L. Al-Madhagi <sup>2</sup> ; A. Pugejs <sup>2</sup> ; S. Schroeder <sup>2</sup> ; <sup>1</sup> University of Leeds/UK; <sup>2</sup> School of Chemical and Process Engineering, University of Leeds/UK |                |
| 13:20   | <b>EFCE PRIZE AWARD LECTURE 2020 / 2021</b><br><b>A Dual Projection System to Characterize Crystallization Processes: Design and Applications</b><br>A.K. Rajagopalan, ETH Zurich/CH  |                |
| 13:45   | <b>Discussion with speakers</b>   |                |
| 14:00   | <b>Closing &amp; Announcement 22<sup>nd</sup> ISIC</b>  |                |
| 14:15   | End of lecture programme  |                |

## Thursday, 2 September 2021

| 14:30 – 17:30   | TUTORIAL C |
|---|------------|
| <b>Modeling, Monitoring and Control of Crystallization Systems</b><br>Z.K. Nagy <sup>1</sup> ; R. Braatz <sup>2</sup> ; E. Simone <sup>3</sup> ; N. Yazdanpanah <sup>4</sup> ; B. Szilagyi <sup>5</sup> ; <sup>1</sup> Loughborough University, Leicestershire/UK and Purdue University/USA; <sup>2</sup> MIT, USA; <sup>3</sup> Leeds University/UK; <sup>4</sup> Procegen/USA; <sup>5</sup> Purdue University/USA |            |



## Thursday, 2 September 2021

| Special Techniques   |  | Virtual Room 3 |
|--|--|----------------|
| <i>Chair: A. Chow, Agency for Science, Technology &amp; Research (A*STAR), Singapore/SGP</i> |  |                |
| 08:30  | <b>Microfluidic-assisted controlled spherical crystallization of Naproxen-Eudragit E100 microparticles</b><br>S. Shikha <sup>1</sup> ; S. Khan <sup>2</sup> ; P. Doyle <sup>3</sup> ; <sup>1</sup> Singapore-MIT Alliance for Research and Technology, Singapore/SGP; <sup>2</sup> National University of Singapore/SGP; <sup>3</sup> Massachusetts Institute of Technology (MIT); Singapore-MIT Alliance for Research and Technology, Cambridge/USA |                |
| 08:50  | <b>Protein Crystallisation with Gas Bubble Templates</b><br>W. Tian <sup>1</sup> ; C. Rielly <sup>1</sup> ; H. Yang <sup>1</sup> ; <sup>1</sup> Loughborough University, Loughborough/UK   |                |
| 09:10  | <b>Pickering Emulsion Assisted Spherical Crystallization of Ibuprofen</b><br>J. Wang <sup>1</sup> ; W. Cao <sup>1</sup> ; L. Zhu <sup>1</sup> ; <sup>1</sup> Zhejiang University of Technology, Hangzhou/CN  |                |
| 09:30  | <b>The integration of membrane emulsification and cooling crystallization of glycine</b><br>S. Kwon <sup>1</sup> ; K. Mathew Thomas <sup>1</sup> ; R. Lakerveld <sup>1</sup> ; <sup>1</sup> The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon/HK  |                |
| 09:50  | <b>Discussion with speakers</b>  |                |
| 10:10  | <b>Coffee Break</b>  |                |
| 10:30  | <b>Poster Session IV</b>   |                |
| 11:30  | <b>Lunch Break</b>   |                |

| Plenary and Keynote Lectures  |  | Virtual Room 1 |
|---|--|----------------|
| <i>Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems &amp; Otto von Guericke University, Magdeburg/D</i> |  |                |
| 12:15   | <b>PLENARY LECTURE</b><br><b>Nucleation theories, 80 years research on nucleation</b><br>H. Cölfen <sup>1</sup> ; <sup>1</sup> Department of Physical Chemistry, University of Konstanz/D  |                |
| 12:55   | <b>KEYNOTE LECTURE</b><br><b>Understanding the Solutions You Crystallise from: The Molecular Basis of Co-solvency and Conformational Changes by X-ray Pair Distribution Function Measurements and Modelling</b><br>A. Pallipurath <sup>1</sup> ; B. Evans <sup>2</sup> ; L. Al-Madhagi <sup>2</sup> ; A. Pugejs <sup>2</sup> ; S. Schroeder <sup>2</sup> ; <sup>1</sup> University of of Leeds/UK; <sup>2</sup> School of Chemical and Process Engineering, University of Leeds/UK |                |
| 13:20   | <b>EFCE PRIZE AWARD LECTURE 2020 / 2021</b><br><b>A Dual Projection System to Characterize Crystallization Processes: Design and Applications</b><br>A.K. Rajagopalan, ETH Zurich/CH   |                |
| 13:45   | <b>Discussion with speakers</b>  |                |
| 14:00   | <b>Closing &amp; Announcement 22<sup>nd</sup> ISIC</b>   |                |
| 14:15   | <b>End of lecture programme</b>  |                |

## Thursday, 2 September 2021

| 14:30 – 17:30  | TUTORIAL C |
|--|------------|
| <b>Modeling, Monitoring and Control of Crystallization Systems</b><br>Z.K. Nagy <sup>1</sup> , R. Braatz <sup>2</sup> , E. Simone <sup>3</sup> , N. Yazdanpanah <sup>4</sup> , B. Szilagy <sup>5</sup> ; <sup>1</sup> Loughborough University, Leicestershire/UK and Purdue University/USA; <sup>2</sup> MIT, USA; <sup>3</sup> Leeds University/UK; <sup>4</sup> Procegen/USA; <sup>5</sup> Purdue University/USA |            |

### POSTER SESSIONS

The poster authors should be ready for poster discussions during the poster sessions. Following topics will be discussed on following dates:

**Monday, 30 August 2021**

**16:25 – 17:30**

#### POSTER SESSION I

**Developments in Large Scale Industrial Crystallization**

P 1.01 – P 1.10

**Contributions of Crystallization to Sustainability**

P 2.01 – P 2.08

**Tuesday, 31 August 2021**

**10:30 – 12:00**

#### POSTER SESSION II

**Fundamentals of Crystallization**

P 3.01 – P 3.49

**Wednesday, 1 September 2021**

**10:30 – 12:00**

#### POSTER SESSION III

**Crystallization & Precipitation in Fine Chemical, Specialty & Life-Science Industries**

P 4.01 – P 4.35

**Thursday, 2 September 2021**

**10:30 – 11:30**

#### POSTER SESSION IV

**Integrated Process Design: Crystallization Process Design in the Industrial Process Chain**

P 5.01 – P 5.15

POSTER SESSION I

Developments in Large Scale Industrial Crystallization

Posters will be discussed on Monday, 30 August 2021

16:25 – 17:30

- P 1.01 **Crystallization process development using Secoy's Crystallization Technology: from lab scale units to a full scale process unit**  
B. Rimez<sup>1</sup>; <sup>1</sup> Secoya technologies, Louvain-la-Neuve/B
- P 1.02 **Population Balance Modeling of Cooling-Antisolvent Crystallization to Derisk Tech-Transfer**  
T. Rosenbaum<sup>1</sup>; L. Tan<sup>1</sup>; N. Mitchell<sup>2</sup>; M. Dummeldinger<sup>1</sup>; J. Engstrom<sup>1</sup>; <sup>1</sup> Bristol-Myers Squibb, New Brunswick/USA; <sup>2</sup> Process Systems Enterprise Limited, London/UK
- P 1.04 **Study of scaling in a plate heat exchanger**  
N. Kamar<sup>1</sup>; M. Le Page Mostefa<sup>1</sup>; H. Muhr<sup>1</sup>; P. Jost<sup>2</sup>; <sup>1</sup> Laboratoire Réaction et Génie des Procédés, Université de Lorraine, Nancy/F; <sup>2</sup> Sofchem, Rueil Malmaison /F
- P 1.05 **Batch crystallization of xylitol by cooling, evaporation and anti-solvent addition**  
A. Zaykovskaya<sup>1</sup>; E. Temmel<sup>2</sup>; M. Stepanski<sup>3</sup>; B. Gevers Deynoot<sup>4</sup>; E. de Jong<sup>4</sup>; M. Louhi-Kultanen<sup>5</sup>; <sup>1</sup> Aalto University School of Chemical Engineering, Espoo/FIN; <sup>2</sup> Sulzer Chemtech Ltd, Allschwil/CH; <sup>3</sup> Sulzer Chemtech Ltd, Winterthur/CH; <sup>4</sup> Avantium, Amsterdam/NL; <sup>5</sup> Aalto University, Espoo/FIN
- P 1.06 **New developments in impeller design for solid-liquid applications**  
B. Nienhaus<sup>1</sup>; <sup>1</sup> EKATO Rühr- und Mischtechnik GmbH, Schopfheim/D
- P 1.07 **A 3D-Printed Low Pressure-Drop Plug-Flow Crystallizer for Protein Crystallization**  
B. Nyande<sup>1</sup>; K. Mathew Thomas<sup>1</sup>; R. Lakerveld<sup>1</sup>; <sup>1</sup> The Hong Kong University of Science and Technology, Hong Kong/HK
- P 1.08 **Ice scaling formation on scraped heat exchanger surfaces during melt/cooling crystallization**  
M. Rodriguez Pascual<sup>1</sup>; D. Xevgenos<sup>2</sup>; <sup>1</sup> Delft University of Technology, Delft/NL; <sup>2</sup> TU Delft/NL
- P 1.09 **Bullet-Proofing Doravirine (MK-1439) Starting Material Supply: Rapid Identification and Response to a New Polymorph of Ethyl Ester**  
P. Larpent<sup>1</sup>; L. Codan<sup>1</sup>; J. Schoell<sup>1</sup>; L. Iuzzolino<sup>2</sup>; M. Tan<sup>2</sup>; J. Newman<sup>2</sup>; A. Lee<sup>2</sup>; <sup>1</sup> MSD Werthenstein BioPharma, Schachen/CH; <sup>2</sup> Merck & Co. Inc., Rahway/USA
- P 1.10 **A novel image analysis technique for 2D characterization of overlapping needle like crystals**  
P. Neoptolemos<sup>1</sup>; <sup>1</sup> The University of Manchester/UK

POSTER SESSION I

Contributions of Crystallization to Sustainability

Posters will be discussed on Monday, 30 August 2021

16:25 – 17:30

- P 2.01 **CaCO<sub>3</sub> precipitation through the carbonation route towards cement industry circular economy**  
F. Liendo Castillo<sup>1</sup>; F. Deorsola<sup>1</sup>; S. Bensaid<sup>1</sup>; <sup>1</sup> Politecnico di Torino, Turin/I
- P 2.02 **-CODA- The Carbon-Negative Soda Ash Project**  
 H. Lorenz<sup>1</sup>; S. Ghaffari<sup>1</sup>; C. Eisenhut<sup>2</sup>; P. Schulze<sup>3</sup>; <sup>1</sup> Max Planck Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; <sup>2</sup> CIECH Soda Deutschland GmbH & Co. KG, Staßfurt/D; <sup>3</sup> SchPrEngCo- Scientific Chemical Process Engineering Consultancy, Magdeburg/D
- P 2.03 **Melt Crystallization of 2,4-Dinitrochlorobenzene: Crystal Growth and Sweating Process Evaluation**  
S. Jia<sup>1</sup>; J. Gong<sup>1</sup>; Z. Gao<sup>1</sup>; J. Wang<sup>1</sup>; <sup>1</sup> Tianjin University/CN
- P 2.04 **CFD-PBM simulation of Mg(OH)<sub>2</sub> precipitation from saltwork brine**  
A. Raponi<sup>1</sup>; <sup>1</sup> Politecnico di Torino, Turin/I
- P 2.05 **Selective in situ product separation by cooling crystallization as a new recycling tool for homogeneous catalysts**  
A. Seifert<sup>1</sup>; A. Laudanski<sup>1</sup>; T. Seidensticker<sup>1</sup>; K. Wohlgemuth<sup>1</sup>; <sup>1</sup> TU Dortmund University, Dortmund/D

- P 2.06 **Understanding Crystallisation in Plant Cuticular Waxes in Relations to Water Permeation through Plant Surfaces**  
L. Parameswaran<sup>1</sup>; K. Roberts<sup>1</sup>; X. Lai<sup>1</sup>; N. George<sup>2</sup>; M. Riederer<sup>3</sup>; <sup>1</sup> University of Leeds/UK;  
<sup>2</sup> Syngenta Crop Protection, Jealott's Hill/UK; <sup>3</sup> Julius Maximilians University of Würzburg/D
- 
- P 2.07 **CFD Study on Heat Transfer in a Layer Melt Crystallizer**  
N. Osmanbegovic<sup>1</sup>; V. Alopaeus<sup>1,2</sup>; V. Vuorinen<sup>1</sup>; M. Louhi-Kultanen<sup>1</sup>; <sup>1</sup> Aalto University School of Chemical Engineering, Espoo/FIN; <sup>2</sup> Aalto University School of Engineering, Espoo/FIN; <sup>2</sup> Department of Chemical Engineering, Mid Sweden University, Sundsvall/S
- 
- P 2.08 **Synthetic BiOBr/Bi<sub>2</sub>S<sub>3</sub>/CdS crystalline material and its degradation of dye under visible light**  
J. Chen<sup>1</sup>; Y. Jin<sup>1</sup>; Z. Xing<sup>1</sup>; Y. Li<sup>1</sup>; J. Han<sup>1</sup>; H. Lorenz<sup>2</sup>; <sup>1</sup> Hebei University of Technology, Tianjin/CN; <sup>2</sup> Max Planck Institute for Dynamics of Complex Technical Systems, Munich/D

### POSTER SESSION II

#### Fundamentals of Crystallization

Posters will be discussed on Tuesday, 31 August 2021

10:30 – 12:00

- P 3.01 **Hierarchical BaCO<sub>3</sub>/SiO<sub>2</sub> Biomorphs: Morphological Evolution & Multi-Functional Development**  
Y. Chen<sup>1</sup>; S. Wang<sup>1</sup>; J. Gong<sup>1</sup>; <sup>1</sup> Tianjin University, Tianjin/CN
- 
- P 3.02 **The development of precipitate characteristics by means of the reactor type and operating conditions**  
M. Stec<sup>1</sup>; P. Synowiec<sup>1</sup>; B. Bunikowska<sup>1</sup>; <sup>1</sup> Silesian University of Technology / Research Network Łukasiewicz, New Chemical Syntheses Institute, Inorganic Chemistry Division "IChN", Gliwice/PL
- 
- P 3.03 **Crystallization of magnesium sulphate heptahydrate from solutions containing calcium and chlorides**  
B. Bunikowska<sup>1</sup>; P. Synowiec<sup>1</sup>; M. Stec<sup>1</sup>; <sup>1</sup> Silesian University of Technology / Research Network Łukasiewicz, New Chemical Syntheses Institute, Inorganic Chemistry Division "IChN", Gliwice/PL
- 
- P 3.04 **Simultaneous crystallization in the ternary system NaCl-Na<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O**  
 A. Sarubbi Lanzotti<sup>1</sup>; M. Martins Seckler<sup>1</sup>; <sup>1</sup> University of São Paulo/BR
- 
- P 3.05 **Thermodynamic based process design for polymers forming different crystalline phases**  
 Z. Fan<sup>1</sup>; S. Enders<sup>2</sup>; M. Fischlschweiger<sup>1</sup>; <sup>1</sup> TU Clausthal / Lehrstuhl für Technische Thermodynamik und Energieeffiziente Stoffbehandlung, Clausthal-Zellerfeld/D; <sup>2</sup> KIT Institut für Technische Thermodynamik und Kältetechnik, Karlsruhe/D
- 
- P 3.06 **Growth of crystal faces tracked in 3D**  
S. Schiele<sup>1</sup>; H. Briesen<sup>1</sup>; <sup>1</sup> TU München, Freising/D
- 
- P 3.07 **Stratification of multi-component solutions on crystalline substrates**  
C. Helfenritter<sup>1</sup>; M. Kind<sup>1</sup>; <sup>1</sup> Karlsruhe Institute of Technology (KIT), Karlsruhe/D
- 
- P 3.08 **Bernoulli offers a solid basis for crystallization**  
H. Meldau<sup>1</sup>; <sup>1</sup> ehemals Sulzer Escher Wyss, Hannover/D
- 
- P 3.09 **Ultrasound-Assisted Crystallization Process Intensification of L-glutamic Acid: Crystal Nucleation and Polymorph Transformation**  
C. Fang<sup>1</sup>; Z. Gao<sup>1</sup>; J. Gong<sup>1</sup>; J. Wang<sup>1</sup>; <sup>1</sup> Tianjin University, Tianjin/CN
- 
- P 3.10 **Controlled Crystallization Process of Potassium Nitrate Solution: Incrustation Phenomenon**  
 M. Al-Rashed<sup>1</sup>; A. Alenzi<sup>1</sup>; A. Mohammad<sup>1</sup>; J. Wójcik<sup>2</sup>; <sup>1</sup> College of Technological Studies, The Public Authority for Applied Education and Training, Shuwaikh/KWT; <sup>2</sup> Silesian University of Technology, Gliwice/PL
- 
- P 3.11 **Implementation of thermal cycling for the control of crystal morphology and size distribution**  
J. Zeglinski<sup>1</sup>; M. Ukrainczyk<sup>1</sup>; G. Morris<sup>1</sup>; B. Glennon<sup>1</sup>; <sup>1</sup> APC Ltd., Dublin/IRL
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- P 3.12 **Thermodynamic description of phase diagrams in solid solution/solvent systems**  
M. Sadeghi<sup>1</sup>; S. Münzberg<sup>1</sup>; V. Tenberg<sup>1</sup>; H. Lorenz<sup>1</sup>; A. Seidel-Morgenstern<sup>2</sup>; <sup>1</sup> Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; <sup>2</sup> Max-Planck-Institut für Dynamik komplexer technischer Systeme & Otto-von-Guericke-Universität Magdeburg, Magdeburg/D
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- P 3.13 **Fluidic Oscillator as a Continuous Crystalliser: Modelling and Validation**  
Y. Yu<sup>1</sup>; A. Pandit<sup>2</sup>; V. Ranade<sup>1</sup>; <sup>1</sup> Queen's University Belfast/UK; <sup>2</sup> Bernal Institute, University of Limerick, Limerick/IRL

- P 3.14 **Crystallizer geometry optimization applying the process model for the Separation of Enantiomers by Preferential Crystallization**  
 N. Huskova<sup>1</sup>; M. Mangold<sup>2</sup>; H. Lorenz<sup>3</sup>; A. Seidel-Morgenstern<sup>3</sup>; <sup>1</sup> Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D; <sup>2</sup> Technische Hochschule Bingen/D; <sup>3</sup> Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D
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- P 3.15 **Modeling crystal growth using the lattice Boltzmann method**  
 Q. Tan<sup>1</sup>; H. Lorenz<sup>2</sup>; S. Hosseini<sup>1</sup>; A. Seidel-Morgenstern<sup>2</sup>; D. Thévenin<sup>1</sup>; <sup>1</sup> OVGU, Magdeburg, Magdeburg/D; <sup>2</sup> Max Planck Institute for Dynamics of Complex Technical Systems (MPI Magdeburg), Magdeburg/D
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- P 3.16 **Strategic Application of Temperature Correction Algorithms for Improved in situ Concentration Monitoring During Cooling Crystallisation**  
 M. Chong<sup>1</sup>; T. McGlone<sup>1</sup>; A. Parrott<sup>1</sup>; A. Nordon<sup>1</sup>; A. Florence<sup>1</sup>; <sup>1</sup> University of Strathclyde, Glasgow/UK
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- P 3.17 **A novel colorimetric experimental technique for the characterization of metal hydroxides reactive crystallization phenomena**  
 S. Romano<sup>1</sup>; G. Battaglia<sup>1</sup>; A. Tamburini<sup>1</sup>; M. Ciofalo<sup>1</sup>; A. Cipollina<sup>1</sup>; G. Micale<sup>1</sup>; <sup>1</sup> Università degli Studi di Palermo/I
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- P 3.18 **Influence of Laser Parameters and Experimental Conditions on Nonphotochemical Laser-Induced Nucleation of Glycine Polymorphs**  
 D. Irimia<sup>1</sup>; J. Jose Shirley<sup>1</sup>; A. Garg<sup>1</sup>; D. Nijland<sup>1</sup>; A. van der Heijden<sup>1</sup>; H. Kramer<sup>1</sup>; H. Eral<sup>1</sup>; <sup>1</sup> Delft University of Technology, Delft/NL
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- P 3.19 **Semi-Batch Evaporation Crystallization for Cobalt Sulfate Recovery**  
 J. Zhang<sup>1</sup>; A. Said<sup>1</sup>; B. Han<sup>1</sup>; M. Louhi-Kultanen<sup>1</sup>; <sup>1</sup> Aalto University, Espoo/FIN
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- P 3.20 **Impact of the phase transition phenomenon of a UCST-type thermoresponsive polymers onto the crystallization of inorganic salts**  
 E. Wong Munoz<sup>1</sup>; M. Lemanowicz<sup>1</sup>; A. Mielańczyk<sup>1</sup>; K. Kiraga<sup>1</sup>; A. Gierczycki<sup>1</sup>; <sup>1</sup> Silesian University of Technology, Gliwice/PL
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- P 3.21 **Time-Resolved X-ray Phase-Contrast Imaging of Continuous Anti-Solvent Crystallisation**  
 G. Das<sup>1</sup>; A. Pallipurath<sup>2</sup>; T. Kathyola<sup>2</sup>; J. Leng<sup>2</sup>; S. Marathe<sup>3</sup>; C. Rau<sup>3</sup>; J. McGinty<sup>4</sup>; R. Miller<sup>4</sup>; J. Sefcik<sup>4</sup>; S. Schroeder<sup>2</sup>; <sup>1</sup> School of Chemical and Process Engineering, University of Leeds/UK; <sup>2</sup> University of Leeds/UK; <sup>3</sup> Diamond Light Source, Didcot/UK; <sup>4</sup> University of Strathclyde/ CMAC, Glasgow/UK
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- P 3.22 **Thermodynamics of Co-Crystal Formation: Estimating the Stability of Sulfamethazine Co-Crystals**  
 M. Svärd<sup>1</sup>; D. Ahuja<sup>2</sup>; <sup>1</sup> KTH Royal Institute of Technology, Stockholm/S; <sup>2</sup> University of Limerick, Limerick/IRL
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- P 3.23 **Precipitation of calcium oxalate in a multifunctional reactor**  
 A. Matysiak<sup>1</sup>; S. Musial<sup>1</sup>; P. Polak<sup>1</sup>; <sup>1</sup> Silesian University of Technology, Gliwice/PL
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- P 3.24 **Application of image analysis methods to enhance crystal shape identification and face indexing**  
 F. Luxenburger<sup>1</sup>; E. Elts<sup>1</sup>; H. Briesen<sup>1</sup>; <sup>1</sup> Lehrstuhl für Systemverfahrenstechnik, TU München, Freising/D
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- P 3.25 **Effect of solvents on crystal size distribution in ultrasound assisted crystallization of ascorbic acid**  
 J. Yadav<sup>1</sup>; S. Patel<sup>1</sup>; <sup>1</sup> Indian Institute of Technology Ropar, Ropar/IND
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- P 3.26 **Experimental Investigation of an Integrated Crystallization and Wet-Milling System with Temperature Cycling to Control the Size and Aspect Ratio of Needle-Shaped Pharmaceutical Crystals**  
 A. Eren<sup>1</sup>; B. Szilágyi<sup>1</sup>; J. Quon<sup>2</sup>; C. Papageorgiou<sup>2</sup>; Z. Nagy<sup>1</sup>; <sup>1</sup> Purdue University, Lafayette/USA; <sup>2</sup> Takeda Pharmaceuticals International Co., Cambridge/USA
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- P 3.27 **Approaches to drying Active Pharmaceutical Ingredients**  
 E. Keavney<sup>1</sup>; B. Wood<sup>2</sup>; A. Healy<sup>1</sup>; B. Glennon<sup>2</sup>; <sup>1</sup> Trinity College Dublin, The University of Dublin/IRL; <sup>2</sup> APC Ltd., Dublin/IRL
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- P 3.28 **Reverse antisolvent crystallization using membrane pervaporation: application to L-Glutamic Acid**  
 M. Khellaf<sup>1</sup>; C. Charcosset<sup>1</sup>; D. Mangin<sup>1</sup>; E. Chabanon<sup>1</sup>; <sup>1</sup> LAGEPP/University of Claude Bernard Lyon 1, Villeurbanne/F
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- P 3.29 **Model-driven Controller Design for Continuous Crystallisation of  $\alpha$ -Lactose Monohydrate**  
 J. Johnston<sup>1</sup>; C. Brown<sup>1</sup>; A. Florence<sup>1</sup>; <sup>1</sup> CMAC/University of Strathclyde, Glasgow/UK
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- P 3.30 **1D and 2-D population balance models applied to mefenamic acid solution crystallisation using gFORMULATE**  
 W. Li<sup>1</sup>; B. Benyahia<sup>1</sup>; C. Rielly<sup>1</sup>; <sup>1</sup> Loughborough University, Loughborough/UK

- P 3.31 **Microfluidics set-up rapidly measures solubility directly from powder**  
G. Peybernes<sup>1</sup>; R. Grossier<sup>1</sup>; F. Villard<sup>2</sup>; P. Letellier<sup>2</sup>; N. Candoni<sup>1</sup>; S. Veester<sup>1</sup>; <sup>1</sup> Aix-Marseille University & CNRS, CINaM, Marseille/F; <sup>2</sup> Technologie Servier, Orléans/F
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- P 3.32 **Template-assisted protein crystallization in microfluidics**  
D. Powell<sup>1</sup>; C. Gerard<sup>1</sup>; M. Briuglia<sup>1</sup>; S. Morais<sup>2</sup>; D. Lamprou<sup>3</sup>; J. Salmon<sup>2</sup>; J. ter Horst<sup>1</sup>; <sup>1</sup> University of Strathclyde/CMAC, Glasgow/UK; <sup>2</sup> CNRS, Université de Bordeaux, Institut de Chimie de la Matière Condensée de Bordeaux, Bordeaux/F; <sup>3</sup> Queens University Belfast/UK
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- P 3.33 **Design and validation of a droplet based microfluidic system to study non-photochemical laser induced nucleation**  
V. Korede<sup>1</sup>; F. Penha<sup>2</sup>; D. Irimia<sup>1</sup>; L. Stam<sup>1</sup>; V. Munck<sup>1</sup>; A. Heijden<sup>1</sup>; H. Kramer<sup>1</sup>; H. Eral<sup>1</sup>; <sup>1</sup> Delft University of Technology, Delft/NL; <sup>2</sup> KTH Royal Institute of Technology, Stockholm/S
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- P 3.34 **Primary and Secondary Nucleation of Sodium Chloride from Water and Deuterium Oxide**  
J. Flannigan<sup>1</sup>; M. Haw<sup>2</sup>; H. Jolliffe<sup>3</sup>; J. Sefcik<sup>1</sup>; <sup>1</sup> EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, c/o Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; <sup>2</sup> Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; <sup>3</sup> EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, c/o Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, Technology and Innovation Centre, Glasgow/UK
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- P 3.35 **Phase Transformation among Multiple Hydrates of Creatine Phosphate Sodium in Solution and in the Vapor**  
J. Dai<sup>1</sup>; L. Zhou<sup>1</sup>; Q. Yin<sup>1</sup>; <sup>1</sup> Tianjin University, Tianjin/CN
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- P 3.36 **Exploring laser induced thermocavitation for primary nucleation control**  
N. Nagalingam<sup>1</sup>; D. Irimia<sup>1</sup>; R. Hartkamp<sup>1</sup>; J. Padding<sup>1</sup>; H. Eral<sup>1</sup>; <sup>1</sup> Delft University of Technology, Delft/NL
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- P 3.37 **Modelling of Turbulent Precipitation in a T-mixer with a Coupled DNS-PBE Approach**  
H. Tang<sup>1</sup>; S. Rigopoulos<sup>1</sup>; G. Papadakis<sup>1</sup>; <sup>1</sup> Imperial College London/UK
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- P 3.38 **Tuning Interface Interactions to Facilitate Heterogeneous Nucleation**  
D. McKechnie<sup>1</sup>; P. Mulheran<sup>1</sup>; J. Sefcik<sup>1</sup>; K. Johnston<sup>1</sup>; <sup>1</sup> University of Strathclyde, Glasgow/UK
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- P 3.39 **The role of pre-nucleation clusters in the crystallization of gold nanoparticles**  
R. Ramamoorthy<sup>1</sup>; E. Yildirim<sup>2</sup>; P. Roblin<sup>1</sup>; L. Lacroix<sup>2</sup>; I. Rodriguez-Ruiz<sup>1</sup>; G. Viau<sup>2</sup>; S. Teychené<sup>1</sup>; <sup>1</sup> INP - ENSIACET - Ecole Nationale Supérieure des Ingénieurs en Arts Chimiques Et Technologiques, Toulouse/F; <sup>2</sup> INSA Toulouse, Toulouse/F
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- P 3.40 **Unveiling the importance of solution structure on the nucleation and the final morphology of gold nanoparticles by using an ultra-fast micro-mixer in coupling with SAXS**  
R. Ramamoorthy<sup>1</sup>; E. Yildirim<sup>2</sup>; P. Roblin<sup>1</sup>; L. Lacroix<sup>2</sup>; I. Rodriguez-Ruiz<sup>1</sup>; A. Diaz<sup>3</sup>; G. Viau<sup>2</sup>; S. Teychené<sup>1</sup>; <sup>1</sup> INP - ENSIACET - Ecole Nationale Supérieure des Ingénieurs en Arts Chimiques Et Technologiques, Toulouse/F; <sup>2</sup> INSA Toulouse, Toulouse/F; <sup>3</sup> Paul Scherrer Institute, Villigen/CH
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- P 3.41 **Towards a rigorous representation of API crystallization kinetics for enabling advanced analysis and comparison**  
G. Lunardon Quillo<sup>1</sup>; S. Bhonsale<sup>2</sup>; B. Gielen<sup>1</sup>; J. Van Impe<sup>2</sup>; A. Collas<sup>1</sup>; C. Xiouras<sup>1</sup>; <sup>1</sup> Janssen Research & Development, Beerse/B; <sup>2</sup> KU Leuven, Ghent/B
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- P 3.42 **Detection of concentration enhancements at nanoscale interfaces**  
R. Mackay<sup>1</sup>; D. McKechnie<sup>1</sup>; K. Johnston<sup>2</sup>; K. Lau<sup>3</sup>; J. Sefcik<sup>1</sup>; <sup>1</sup> EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, c/o Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; <sup>2</sup> Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; <sup>3</sup> University of Strathclyde, Glasgow/UK
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- P 3.43 **On the possible stereoselectivity of Non-Photochemical Laser Induced Nucleation**  
M. Briard<sup>1</sup>; C. Brandel<sup>1</sup>; V. Dupray<sup>1</sup>; G. Coquerel<sup>1</sup>; <sup>1</sup> Normandie Université, Rouen/F
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- P 3.44 **Solubility and Nucleation Kinetics of a Homologous Series of 8 Representative Diesel n-Alkanes (C<sub>16</sub> – C<sub>23</sub>) in Toluene & Dodecane**  
A. Jackson<sup>1</sup>; K. Roberts<sup>1</sup>; R. Downie<sup>2</sup>; P. Dowding<sup>2</sup>; <sup>1</sup> University of Leeds, Leeds/UK; <sup>2</sup> Infineum UK Ltd., Abingdon/UK
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- P 3.45 **Predicting temperature dependent solubility from thermodynamic data measured at a single temperature: Application to glycine polymorphs**  
A. Manson<sup>1</sup>; L. Lue<sup>1</sup>; J. Sefcik<sup>1</sup>; <sup>1</sup> University of Strathclyde, Glasgow/UK

- P 3.46 **Determining the solubility of  $Y_2(SO_4)_3$  in  $H_2O-C_nH_{2n+1}OH$  systems for the recovery of rare earth elements using antisolvent crystallization.**  
J. Du Plessis<sup>1</sup>; J. Chivavava<sup>1</sup>; A. Lewis<sup>1</sup>; <sup>1</sup> University of Cape Town, Cape Town/ZA
- P 3.47 **Modeling kinetics of secondary nucleation facilitated by inter-particle energies**  
B. Ahn<sup>1</sup>; L. Bosetti<sup>1</sup>; M. Mazzotti<sup>1</sup>; <sup>1</sup> ETH Zurich/CH
- P 3.48 **Predicting relative solubilities with molecular dynamics simulations**  
Z. Bjelobrk<sup>1</sup>; D. Mendels<sup>2</sup>; T. Karmakar<sup>3</sup>; M. Parrinello<sup>3</sup>; M. Mazzotti<sup>1</sup>; <sup>1</sup> ETH Zurich/CH; <sup>2</sup> University of Chicago, Illinois/USA; <sup>3</sup> Istituto Italiano di Tecnologia, Genova/I
- P 3.49 **Insights into Intermolecular Interactions of Spironolactone Solvates**  
L. Jia<sup>1</sup>; L. Zhou<sup>2</sup>; Q. Yin<sup>2</sup>; <sup>1</sup> Tianjin University, Tianjin/CN

### POSTER SESSION III

#### Crystallization & Precipitation in Fine Chemical, Specialty & Life-Science Industries

Posters will be discussed on Wednesday, 1 September 2021, 10:30 – 12:00

- P 4.01 **Difference in particle morphology of betamethasone by the addition of bio-surfactant between spray-drying and freeze-drying**  
K. Kadota<sup>1</sup>; H. Uchiyama<sup>1</sup>; Y. Tozuka<sup>1</sup>; <sup>1</sup> Osaka University of Pharmaceutical Sciences, Osaka/J
- P 4.02 **Solid phases relations and thermal deformations of L-serine and L-alanine**  
R. Sadovnichii<sup>1</sup>; L. Kryuchkova<sup>1</sup>; E. Kotelnikova<sup>1</sup>; H. Lorenz<sup>2</sup>; <sup>1</sup> St. Petersburg State University, St. Petersburg/RUS; <sup>2</sup> Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D
- P 4.03 **The Continuous Operation of Parallel Placed Tubular Micro-Nucleators**  
B. Rimez<sup>1</sup>; <sup>1</sup> Secoya technologies, Louvain-la-Neuve/B
- P 4.04 **Production scale supersaturation control from production manager's point of view**  
L. Simon<sup>1</sup>; P. Emery<sup>2</sup>; J. Webb<sup>3</sup>; Y. Elias<sup>4</sup>; Z. Nagy<sup>5</sup>; J. Hone<sup>3</sup>; K. Hungerbühler<sup>4</sup>; <sup>1</sup> Syngenta Crop Protection AG, Münchwilen/CH; <sup>2</sup> Syngenta Crop Protection AG, Muenchwilen/CH; <sup>3</sup> Syngenta Crop Protection, Jealots-Hill/UK; <sup>4</sup> ETH Zurich/CH; <sup>5</sup> Loughborough University, Loughborough/UK
- P 4.05 **On the Similitude of Technical Precipitation**  
H. Rehage<sup>1</sup>; J. Orthey<sup>1</sup>; M. Kind<sup>1</sup>; <sup>1</sup> Karlsruhe Institute of Technology (KIT), Karlsruhe/D
- P 4.06 **TBD - Pending legal review**  
N. Mitchell<sup>1</sup>; J. Webb<sup>2</sup>; R. Taylor<sup>3</sup>; K. Foster<sup>2</sup>; S. Ward-Smith<sup>3</sup>; P. Kippax<sup>3</sup>; O. Lobanova<sup>2</sup>; A. Collier<sup>2</sup>; A. Salmon<sup>1</sup>; <sup>1</sup> PSE - A Siemens Business, London/UK; <sup>2</sup> Syngenta, Bracknell/UK; <sup>3</sup> Malvern Panalytical Ltd., Malvern/UK
- P 4.07 **Preparation of mesoporous calcium carbonate by crystallization processing**  
S. Yamanaka<sup>1</sup>; K. Sridhar<sup>1</sup>; K. Kadota<sup>2</sup>; H. Uchiyama<sup>2</sup>; Y. Tozuka<sup>2</sup>; Y. Yusof<sup>3</sup>; <sup>1</sup> Muroran Institute of Technology, Muroran/J; <sup>2</sup> Osaka University of Pharmaceutical Sciences, Takatsuki/J; <sup>3</sup> Universiti Putra Malaysia, Selangor/MAL
- P 4.08 **Achieving particle size and impurity control for a continuous crystallization and wet milling process using a digital design approach**  
N. Mitchell<sup>1</sup>; C. Burcham<sup>2</sup>; F. Calado<sup>1</sup>; S. Myers<sup>2</sup>; S. Pereira<sup>1</sup>; <sup>1</sup> PSE - A Siemens Business, London/UK; <sup>2</sup> Eli Lilly and Company, Indianapolis/USA
- P 4.09 **pH-sensitive polymethacrylate derivatives Eudragit E100 & L100 nanoparticles preparation in aqueous medium**  
F. Ofridam<sup>1</sup>; N. Lebaz<sup>1</sup>; E. Gagnière<sup>1</sup>; D. Mangin<sup>1</sup>; A. Elaissari<sup>2</sup>; <sup>1</sup> University Claude Bernard Lyon-1/ CNRS, LAGEPP-UMR 5007, Villeurbanne/F; <sup>2</sup> University Claude Bernard Lyon-1/ CNRS, ISA-UMR 5280, Villeurbanne/F
- P 4.10 **Towards enhanced understanding of sono-crystallization for pharmaceuticals**  
D. Pohlman<sup>1</sup>; M. Boukerche<sup>2</sup>; H. Shariff<sup>3</sup>; N. Nere<sup>4</sup>; <sup>1</sup> Abbvie, North Chicago/USA; <sup>2</sup> Process Research And Development/AbbVie Inc., Chicago/USA; <sup>3</sup> Missouri University of Science and Technology, Rolla, MO/USA; <sup>4</sup> AbbVie Inc., North Chicago/USA
- P 4.11 **Extending the scope of impedance spectroscopy as a PAT-tool during crystallization**  
C. Eder<sup>1</sup>; H. Briesen<sup>1</sup>; <sup>1</sup> Technical University of Munich, Freising/D

- P 4.12 **Using solvent additives in melt crystallization of high-viscous organic mixtures**  
M. Ila<sup>1</sup>; M. Louhi-Kultanen<sup>1</sup>; E. Temmel<sup>2</sup>; M. Stepanski<sup>3</sup>; J. Singh<sup>4</sup>; B. Gevers Deynoot<sup>4</sup>; E. de Jong<sup>4</sup>; <sup>1</sup> Aalto University, Espoo/FIN; <sup>2</sup> Sulzer Chemtech Ltd., Allschwil/CH; <sup>3</sup> Sulzer Chemtech Ltd., Winterthur/CH; <sup>4</sup> Avantium, Amsterdam/NL
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- P 4.13 **Understanding the relationship between the crystal structure of different solid forms of quercetin and their physical properties using synthonic modelling**  
P. Klitou<sup>1</sup>; I. Rosbottom<sup>1</sup>; E. Simone<sup>1</sup>; <sup>1</sup> University of Leeds/UK
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- P 4.14 **Experimental characterisation and population balance modelling of batch cooling crystallisation of hexamine in ethanol**  
R. Leeming<sup>1</sup>; T. Mahmud<sup>1</sup>; K. Roberts<sup>1</sup>; E. Simone<sup>1</sup>; N. George<sup>2</sup>; <sup>1</sup> University of Leeds/UK; <sup>2</sup> Syngenta, Bracknell/UK
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- P 4.15 **Comparison of Isolation-Free Continuous Crystallization Operations: Falling Film Solution Layer Crystallization and Confined Suspension Crystallization**  
R. Lopez-Rodriguez<sup>1</sup>; M. Harding<sup>1</sup>; G. Gibson<sup>2</sup>; K. Girard<sup>3</sup>; S. Ferguson<sup>1</sup>; <sup>1</sup> University College Dublin, Dublin/IRL; <sup>2</sup> Pfizer Limited, Cork/IRL; <sup>3</sup> Pfizer Inc. Worldwide Research and Development, Groton/USA
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- P 4.16 **Analysis of the Crystallisation Behaviour of the Diastereomer System of DL-arabinose and DL-xylose**  
B. Tyson<sup>1</sup>; C. Pask<sup>1</sup>; N. George<sup>2</sup>; E. Simone<sup>1</sup>; <sup>1</sup> University of Leeds/UK; <sup>2</sup> Syngenta, Jealotts Hill/UK
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- P 4.17 **Separation strategies for valorization of lignin by targeted molecular weight fractionation**  
A. Ponnudurai<sup>1</sup>; P. Schulze<sup>1</sup>; A. Seidel-Morgenstern<sup>2</sup>; <sup>1</sup> Max Planck Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; <sup>2</sup> Max Planck Institut für Dynamik komplexer technischer Systeme / Otto-von-Guericke Universität Magdeburg/D
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- P 4.18 **Digital design of a robust continuous crystallization process: Using mechanistic modelling tools to minimize material requirements at the R&D stage**  
B. Mehta<sup>1</sup>; C. Brown<sup>2</sup>; N. Mitchell<sup>1</sup>; B. Williams<sup>1</sup>; <sup>1</sup> PSE - A Siemens Business, London/UK; <sup>2</sup> University of Strathclyde, Glasgow/UK
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- P 4.19 **Reactive crystallization kinetics of K<sub>2</sub>SO<sub>4</sub> from picromerite-based MgSO<sub>4</sub> and KCl**  
A. Albis<sup>1</sup>; H. Lorenz<sup>2</sup>; Y. Jiménez<sup>3</sup>; T. Graber<sup>3</sup>; <sup>1</sup> Universidad de Antofagasta/RCH; <sup>2</sup> Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D; <sup>3</sup> Universidad de Antofagasta/RCH
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- P 4.20 **Sonochemical Synthesis of Double Salt Compound**  
S. Kamei<sup>1</sup>; M. Matsumoto<sup>2</sup>; S. Furukawa<sup>1</sup>; <sup>1</sup> Nihon University, Izumi-cho, Narashino, Chiba/J; <sup>2</sup> Nihon University, Shinnei, Narashino, Chiba/J
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- P 4.21 **Continuous chiral resolution by diastereomeric salt formation of racemic Ibuprofen in a Couette-Taylor crystallizer**  
L. Marc<sup>1</sup>; J. Schneider<sup>2</sup>; G. Coquerel<sup>1</sup>; <sup>1</sup> Université de Rouen Normandie, Mont-Saint-Aignan/F; <sup>2</sup> Seqens, Porcheville/F
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- P 4.22 **Thermal deformations of the crystal structures of L-aspartic, DL-aspartic and β-L-glutamic amino acids**  
R. Sadovnichii<sup>1</sup>; H. Lorenz<sup>2</sup>; E. Kotelnikova<sup>1</sup>; <sup>1</sup> Sant Petersburg State University, Saint Petersburg/RUS; <sup>2</sup> Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D
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- P 4.23 **Crystallization-based Purification of Multicomponent Plant Extracts: The Case Study of Artemisinin**  
S. Wünsche<sup>1</sup>; S. Triemer<sup>1</sup>; G. Vu<sup>1</sup>; A. Seidel-Morgenstern<sup>2</sup>; H. Lorenz<sup>1</sup>; <sup>1</sup> Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; <sup>2</sup> Max-Planck-Institut für Dynamik komplexer technischer Systeme & Otto-von-Guericke-Universität, Magdeburg/D
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- P 4.24 **Control of impurity profile and crystal morphology through crystallisation process design**  
A. Jawor-Baczynska<sup>1</sup>; L. Agnew<sup>1</sup>; G. Howell<sup>1</sup>; N. Adlington<sup>1</sup>; <sup>1</sup> AstraZeneca Macclesfield, Macclesfield/UK
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- P 4.25 **Characterization of a Small-Scale Crystallizer using Multiphase CFD Simulations and X-Ray Tomography Measurements**  
R. Achermann<sup>1</sup>; R. Adams<sup>1</sup>; H. Prasser<sup>1</sup>; M. Mazzotti<sup>1</sup>; <sup>1</sup> ETH Zurich/CH
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- P 4.26 **A Selective Dissolution Process Featuring a Hydrocyclone for the Removal of Fines in Crystallization**  
P. Binel<sup>1</sup>; <sup>1</sup> ETH Zurich/CH
- 
- P 4.27 **Seeded batch protein crystallization in a meso oscillatory flow reactor**  
F. Castro<sup>1</sup>; A. Ferreira<sup>1</sup>; J. Teixeira<sup>2</sup>; F. Rocha<sup>1</sup>; <sup>1</sup> Faculty of Engineering - University of Porto/P; <sup>2</sup> University of Minho, Braga/P



## POSTER PROGRAMME

- P 4.29 **A Contribution to the Melt Phase Diagram and Solid-State Forms of Chiral Drug Aminoglutethimide**  
B. Saikia<sup>1</sup>; F. Cascella<sup>2</sup>; A. Seidel-Morgenstern<sup>1</sup>; H. Lorenz<sup>1</sup>; <sup>1</sup> Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D
- P 4.30 **Beyond Structure Determination: Crystallisation as a Purification Unit Process for Proteins and Peptides**  
I. Rosbottom<sup>1</sup>; F. Link<sup>1</sup>; W. Chen<sup>1</sup>; N. Mitchell<sup>2</sup>; J. Heng<sup>1</sup>; <sup>1</sup> Imperial College London, London/UK; <sup>2</sup> PSE - A Siemens Business, London/UK
- P 4.31 **Insights on the formation and dissociation mechanisms of cyclopentane hydrate obtained by using calorimetry and optical microscopy**  
R. Ramamoorthy<sup>1</sup>; J. Torr  <sup>1</sup>; I. Rodriguez-Ruiz<sup>2</sup>; S. Teychen  <sup>1</sup>; <sup>1</sup> INP - ENSIACET - Ecole Nationale Sup  rieure des Ing  nieurs en Arts Chimiques Et Technologiques, Toulouse/F
- P 4.32 **A novel strategy for deracemization using periodic fluctuations of supersaturation**  
K. Intaraboonrod<sup>1</sup>; A. Flood<sup>2</sup>; <sup>1</sup> Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong/T; <sup>2</sup> VISTEC, Rayong/T
- P 4.33 **Effects of crystallization conditions on the physical properties of cocoa butter – based oleofoams: a multi-technique approach**  
L. Metilli<sup>1</sup>; M. Holmes<sup>1</sup>; M. Povey<sup>1</sup>; A. Lazidis<sup>2</sup>; S. Marty-Terrade<sup>2</sup>; J. Ray<sup>3</sup>; E. Simone<sup>1</sup>; <sup>1</sup> University of Leeds/UK; <sup>2</sup> Nestl   Product Technology Centre Confectionery York, York/UK; <sup>3</sup> Nestl   Research Vers-chez-les-Blanc, Lausanne/CH
- P 4.34 **Flow-driven Crystallization of Lithium Phosphate in Microchannels**  
M. Emmanuel<sup>1</sup>; D. Horv  th<sup>1</sup>;   . T  th<sup>1</sup>; <sup>1</sup> University of Szeged/H
- P 4.35 **Investigating Moisture-Induced Crystallisation By Dynamic Vapour Sorption**  
M. Naderi<sup>1</sup>; M. Guo<sup>2</sup>; D. Burnett<sup>3</sup>; <sup>1</sup> Surface Measurement Systems, London/UK; <sup>2</sup> Surface Measurement Systems (SMS), London/UK; <sup>3</sup> Surface Measurement Systems (SMS), Allentown/USA

### POSTER SESSION IV

#### Integrated Process Design: Crystallization Process Design in the Industrial Process Chain

Posters will be discussed on Thursday, 2 September 2021

10:30 – 11:30

- P 5.01 **Workflow Towards Melt Crystallization Process Design in Specialty Chemistry**  
M. L  hrmann<sup>1</sup>; S. Schr  der<sup>1</sup>; L. Hohmann<sup>1</sup>; <sup>1</sup> Evonik Operations GmbH | Technology & Infrastructure, Marl/D
- P 5.02 **Selection of continuous crystallization technologies within a process design methodology**  
A. Schindel<sup>1</sup>; M. Polyakova<sup>1</sup>; M. Gr  newald<sup>1</sup>; <sup>1</sup> Ruhr-Universit  t Bochum/D
- P 5.03 **Precipitation of Cu/ZnO on a quasi-continuous filter belt apparatus**  
S. H  ving<sup>1</sup>; B. Nierhauve<sup>1</sup>; N. Kockmann<sup>1</sup>; <sup>1</sup> TU Dortmund University, Dortmund/D
- P 5.04 **Digital design of end-to-end manufacturing process for mefenamic acid using mechanistic modelling**  
C. Brown<sup>1</sup>; N. Mitchell<sup>2</sup>; F. Doerr<sup>1</sup>; J. McGinty<sup>1</sup>; M. Chong<sup>1</sup>; M. Robertson<sup>1</sup>; S. Ottoboni<sup>1</sup>; W. Li<sup>3</sup>; <sup>1</sup> University of Strathclyde, Glasgow/UK; <sup>2</sup> Process Systems Enterprise, London/UK; <sup>3</sup> Loughborough University, Loughborough/UK
- P 5.05 **Using modelling tools to accelerate the design process of the innovative continuous Archimedes tube crystallizer**  
J. Sonnenschein<sup>1</sup>; R. Heming<sup>1</sup>; M. Aghayarzadeh<sup>1</sup>; O. Mierka<sup>1</sup>; S. Turek<sup>1</sup>; G. Schembecker<sup>1</sup>; K. Wohlgemuth<sup>1</sup>; <sup>1</sup> TU Dortmund University, Dortmund/D
- P 5.06 **Impact of Operating Parameters on Continuous Slug Flow Crystallization**  
A. Kufner<sup>1</sup>; M. Term  hlen<sup>1</sup>; K. Wohlgemuth<sup>1</sup>; <sup>1</sup> TU Dortmund University, Dortmund/D
- P 5.07 **Designing a Continuous Taylor-Couette Crystallizer – Residence Time Distribution and Suspension Characteristics**  
M. Etmanski<sup>1</sup>; M. Breloer<sup>1</sup>; G. Schembecker<sup>1</sup>; K. Wohlgemuth<sup>1</sup>; <sup>1</sup> TU Dortmund University, Dortmund/D
- P 5.08 **New soft sensor design for a batch crystallization process based on solute concentration**  
L. Brivadis<sup>1</sup>; V. Andrieu<sup>1</sup>;   . Chabanon<sup>1</sup>; E. Gagnier  <sup>1</sup>; N. Lebaz<sup>1</sup>; U. Serres<sup>1</sup>; <sup>1</sup> Universit   Lyon 1, Laboratoire d'Automatique et de G  nie des Proc  d  s, UMR 5007, CNRS–ESCPE, Villeurbanne/F
- P 5.09 **New inversion method for the multi-shape CLD-to-PSD problem with spheroid particles**  
L. Brivadis<sup>1</sup>; L. Sacchelli<sup>1</sup>; <sup>1</sup> Universit   Lyon 1, Laboratoire d'Automatique et de G  nie des Proc  d  s, UMR 5007, CNRS–ESCPE, Villeurbanne/F

- P 5.10 **Digital design of crystallization and Advanced Process Control using mechanistic models**  
J. Mack<sup>1</sup>; R. Parekh<sup>1</sup>; F. Tahir<sup>1</sup>; C. Brown<sup>2</sup>; J. Johnston<sup>2</sup>; J. Robertson<sup>2</sup>; N. Mitchell<sup>3</sup>; A. Florence<sup>2</sup>; <sup>1</sup> Perceptive Engineering - an Applied Materials Company, Daresbury/UK; <sup>2</sup> CMAC/ University of Strathclyde, Glasgow/UK; <sup>3</sup> PSE - A Siemens Business, London/UK
- 
- P 5.11 **Size and Shape Engineering of Needle-like Particles: Process Development and Process Control**  
A. Rajagopalan<sup>1</sup>; S. Bötschi<sup>1</sup>; F. Salvatori<sup>1</sup>; P. Binel<sup>1</sup>; M. Morari<sup>2</sup>; M. Mazzotti<sup>1</sup>; <sup>1</sup> ETH Zurich/CH; <sup>2</sup> University of Pennsylvania, Philadelphia/USA
- 
- P 5.12 **Process Development for Size and Shape Manipulation of plate-like crystals**  
D. Biri<sup>1</sup>; A. Jaeggi<sup>1</sup>; P. Binel<sup>1</sup>; A. Rajagopalan<sup>1</sup>; M. Mazzotti<sup>1</sup>; <sup>1</sup> ETH Zurich/CH
- 
- P 5.13 **A crystallisation development workflow for the manufacturability enhancement/improvement of active pharmaceutical ingredients**  
H. Siddique<sup>1</sup>; <sup>1</sup> CMAC National Facility, Glasgow/UK
- 
- P 5.14 **Model-based optimal choice of pressure-driven withdrawal method from stirred suspensions**  
R. Achermann<sup>1</sup>; V. Wiedmeyer<sup>1</sup>; M. Hosseinalipour<sup>1</sup>; S. Güngör<sup>1</sup>; M. Mazzotti<sup>1</sup>; <sup>1</sup> ETH Zurich/CH
- 
- P 5.15 **Multidimensional particle characterisation from in-situ imaging using deep learning and transfer learning**  
C. Boyle<sup>1</sup>; C. Ferreira<sup>2</sup>; Y. Chen<sup>2</sup>; C. Tachtatzis<sup>3</sup>; I. Andronovic<sup>3</sup>; C. Brown<sup>1</sup>; J. Sefcik<sup>1</sup>; J. Cardona<sup>1</sup>; <sup>1</sup> CMAC Future Manufacturing Research Hub, University of Strathclyde, Glasgow/UK; <sup>2</sup> Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; <sup>3</sup> Department of Electronic and Electrical Engineering, University of Strathclyde, Glasgow/UK

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