

BACG Annual Conference 2022



Sessions' details

Plenary Lecture (10:00 - 10:40) (Chairs: Jan Sefcik and Huaiyu Yang)

Dr Jerry Heng

Title: TBC

Session 1 (Chairs: Jan Sefcik and Huaiyu Yang)

Devis Di Tommaso (10:40 - 11:00):

Solution additives promoting the onset of MgCO_3 nucleation and growth.

Krishna Hari (11:00 - 11:10):

Engineered growth of polycrystalline amino acid films for eco-friendly piezoelectric sensing.

Zoran Bjelobrk (11:10 - 11:20):

Solubility of organic salts in solvent-antisolvent mixtures: A combined experimental and molecular dynamics simulations approach.

Session 2 (Chairs: Petros Neoptolemos and Simon Lawrence)

Ryan Leeming (11:30 - 11:50):

Model predictive control of industrial crystallisation processes.

Mitchelle Kudzanayi Mandaza (11:50 - 12:00):

Digital Design Strategies for Industrial Crystallisation Development: Considering Active Pharmaceutical Ingredient Properties.

Thomas Pickles (12:00 - 12:10):

Developing an autonomous DataFactory workflow for small-scale batch cooling crystallization with the antiviral lamivudine.

Yiming Ma (12:10 - 12:20):

Design of the Cooling Crystallization Process using the Machine Learning-based Strategy.

Young Scientist Talk, Mingxia Guo (13:05 - 13:35) (Chairs: Elena Simone and Petros Neoptolemos)

The role of water in peptide crystallisation and the relationship between peptide conformation and crystallisation conditions.

Session 3 (Chairs: Zarrin Ansari, Weronika Kras and Gareth Lloyd)

Colin Seaton (14:00 - 14:20):

Isostructural Molecular Crystals: Combining Experimental and Computational Screening.

Haibin Qu (14:20 - 14:30):

Prediction Method Development and Formulation Performance Evaluation of Thiophanate-methyl Cocrystals.

Lihong Jia (14:30 - 14:40):

Deep Insights into the Selective Formation of Isostructural Crystal: A Case of Spironolactone Solvates.

Ruiaridh Mackay (14:40 - 14:50):

Measuring Interface Induced Concentration Enhancement in Molecular Mixtures.

Wenqing Tian (14:50 - 15:00):

Protein Crystallisation by Gas Bubbles with In-situ Tracking in a Batch Reactor.

Session 4 (Chairs: Grahame Woollam and Simon Lawrence)

Nathan de Bruyn (15:10 - 15:30):

CrystalGrower: Crystal Shape Prediction, Analysis and Design – a Study of Molecular Crystals.

Samira Anker (15:30 - 15:40):

Controlling urea crystallisation via heterogeneous nucleation.

James Flannigan (15:40 - 15:50):

Crystal Nucleation from Solution Induced by Optical Tweezers.

Steven-Nicholson (15:50 - 16:00):

Measurement of Boundary Layer Concentration Distribution, Thickness and Mass Flux during Growth and Dissolution of the {011} and {120} Faces of L-alanine Single Crystals.

Plenary Lecture (16:10 - 16:50) (Chairs: Grahame Woollam and Simon Lawrence)

Dr Robert Docherty

Digitally Enabled Workflows: Accelerating the Molecule to Medicine Journey