

MSDE Symposium 2021: Frontiers in Molecular Engineering

17 June - 18 June 2021

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Draft Programme

All times shown are British Summer Time (BST).

Thursday 17 June

09:05	Welcome and Introductions Maria Southall <i>Executive Editor of MSDE, Royal Society of Chemistry</i>	
Session 1 Chair: Maria Southall		
09:20	Tanja Junkers <i>Monash University, Australia</i>	Muconic acid esters as bioderived acrylate mimics
09:40	Wen-bin Zhang <i>Peking University, China</i>	Cellular Synthesis of Topological Proteins
10:00	Fei Sun <i>The Hong Kong University of Science and Technology, China</i>	Engineer Biology for New Materials
10:20	Discussion	
10:40	Break and poster session	
Session 2 Chair: Luke Connal		
11:50	Marc-Olivier Coppens <i>University College London, UK</i>	Nature-Inspired Solutions for Molecular Systems Design and Engineering
12:10	Anja Palmans <i>Eindhoven University of Technology, Netherlands</i>	Folding Polymers into Functional Materials
12:30	Seth Darling <i>Argonne National Laboratory, USA</i>	Water Science and Technology by Interface Design
12:50	Discussion	
13:10	Break and poster session	
Session 3 Panel Discussion on polymer upcycling and sustainability Chair: tbc		
14:00	Welcome Juan de Pablo <i>University of Chicago, USA</i>	
14:20	Gregg Beckham <i>National Renewable Energy Laboratory, USA</i> LaShanda Korley <i>University of Delaware, USA</i> Stuart Rowan <i>University of Chicago, USA</i>	

15:20	Break and poster session	
Session 4 Moulton Medal Winners Chair: Linda Broadbelt		
16:00	Introduction from IchemE: Moulton Medal <i>Claudia Flavell-While</i>	
16:10	Randall Snurr <i>Northwestern University, USA</i>	Molecular Simulation and Machine Learning to Rapidly Predict the Adsorption Properties of Metal-Organic Frameworks
16:30	David Danaci <i>Imperial College London, UK</i>	Adsorbent screening tools for post-combustion carbon capture via pressure- and temperature-vacuum swing adsorption
16:50	Carmine D'Agostino <i>University of Manchester, UK</i>	Tailoring morphology of hierarchical catalysts for tuning pore diffusion behaviour: a rational guideline exploiting bench-top pulsed-field gradient (PFG) nuclear magnetic resonance (NMR)
17:10	Discussion	
Session 5 Equity, Diversity, and Inclusion Workshop Chair: Pat Stayton		
17:30	Laura Norton <i>Senior Programme Manager, Inclusion & Diversity, Royal Society of Chemistry</i> Monica R. Hall-Porter <i>Faculty Development Coordinator, Associate Professor of Instruction</i> <i>University of Texas at Austin, USA</i>	
18:30	Final remarks Juan de Pablo <i>University of Chicago, USA</i>	
18:40	Close of Day 1	

Friday 18 June

09:10	Welcome and Introductions Maria Southall <i>Executive Editor of MSDE, Royal Society of Chemistry</i>	
Session 6 Chair: Maria Southall		
09:20	Jacqui Cole <i>University of Cambridge, UK</i>	Data-driven materials discovery of light harvesters for photovoltaic applications
09:40	Nobuhiro Yanai <i>Kyushu University, Japan</i>	Upconverting sunlight and indoor light to create UV light
10:00	Discussion	
10:20	Break	
Session 7 Chair: Luke Connal		
11:00	Siddharth V. Patwardhan <i>University of Sheffield, UK</i>	Designing bioinspired green nanosilicas using statistical and machine learning approaches
11:20	Caroline Mellot-Draznieks <i>Collège de France, France</i>	POM@MOF composites for CO ₂ reduction : Combining solid state

		NMR, PDF and DFT calculations for rationalizing photocatalytic activities
11:40	Discussion	
12:00	Break and poster session	
Session 8		
Chair: Andrew Fergusson		
14:00	Psaras McGrier <i>Ohio State University, USA</i>	Covalent Organic Frameworks for Catalytic and Energy Storage Applications
14:20	Ying Diao <i>University of Illinois at Urbana-Champaign, USA</i>	Chiral emergence during hierarchical assembly of achiral conjugated polymers
14:40	Discussion	
Session 9		
Chair: Claire Adjiman		
15:00	Darrin Pochan <i>University of Delaware, USA</i>	Biomaterials for non-biological things
15:20	Lola Eniola-Adefeso <i>University of Michigan, USA</i>	A Gold-Templated Method for Fabrication of Bile Salt-Based Composite Microparticles
15:40	Discussion	
16:00	Break	
Session 10		
MSDE Early Career Award Winners		
Chair: Maria Southall		
16:10	MSDE Early Career Award Introduction Maria Southall <i>Executive Editor of MSDE, Royal Society of Chemistry</i>	
16:20	Jodie Lutkenhaus <i>Texas A&M University, USA</i>	
16:40	Heather Kulik <i>MIT, USA</i>	What problems can machine learning solve in transition metal complex discovery?
17:00	Discussion	
17:20	Poster Award Presentation Bianca Provost <i>Deputy Editor of MSDE, Royal Society of Chemistry</i>	
17:30	Final Remarks Juan de Pablo <i>University of Chicago, USA</i>	
17:35	Close of day 2	

Please note that this is a draft programme and timings may change. Please contact the event organisers at kerrh@rsc.org to request changes to the programme.

