

CHEMICAL SCIENCE SYMPOSIUM 2020

How can machine learning and autonomy accelerate chemistry?

29 – 30 September 2020
Online event

Day 1 (Times given for UK BST)

13:00	Welcome and introduction to day 1
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Session 1: Chair - Alán Aspuru-Guzik *University of Toronto, Canada*

13:10	Efficient exploration of solid state chemical space using machine learning Yousung Jung <i>KAIST, South Korea</i>	Inv. 1
13:30	Building a computational engine to guide the autonomous discovery of molecular materials Graeme Day <i>University of Southampton, UK</i>	Inv. 2
13:50	Session 1 discussion	
14:20	Break	

Session 2: Chair - Luis Campos *Columbia University, USA*

14:35	Autonomous materials discovery: promise, pitfalls, and progress Joshua Schrier <i>Fordham University, USA</i>	Inv. 3
14:55	Accelerating materials innovation: discovery of electrochromic materials for smart windows Jill Becker <i>Kebotix, USA</i>	Inv. 4
15:15	Session 2 discussion	
15:45	Break	

Poster Session & Networking Rooms

16:00	Poster session 1	General networking	Networking Sessions 1	
16:30				Networking Sessions 2
17:00				
17:30	Close			

Day 2 (Times given for UK BST)

12:00	Welcome and introduction to day 2
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Session 3: Chair - Kim Jelfs *Imperial College London, UK*

12:10	Accelerating materials discovery with data mining and machine learning Jacqueline Cole <i>University of Cambridge, UK</i>	Inv. 5
12:30	The chemical oracle Lee Cronin <i>University of Glasgow, UK</i>	Inv. 6
12:50	Session 3 discussion	
13:20	Break	

Poster Session & Networking Rooms

13:20	Poster session 2	General networking	
13:35			Networking Sessions 3
14:05			

Session 4: Chair - Andrei Yudin *University of Toronto, Canada*

14:20	Suitable automation systems for accelerating chemical research Kerstin Thurow <i>University of Rostock, Germany</i>	Inv. 7
14:40	Autonomous chemical synthesis in flow for drug discovery María José Nieves Remacha <i>Eli Lilly and Company, Spain</i>	Inv. 8
15:00	Session 4 discussion	
15:30	Closing remarks and poster awards	
15:45	Close of symposium	