

## Leverhulme Research Centre for Functional Materials Design 3<sup>rd</sup> Biennial Materials Symposium

**PROGRAMME: Tuesday 12<sup>th</sup> November 2024**

09.00 – 10.00	<b>Registration and Coffee</b>
10.00 – 10.15	<b>Welcome &amp; Intro to the LRC</b> Prof. Andrew I Cooper Director, Leverhulme Research Centre for Functional Materials Design
<b>Session 1: <span style="float: right;">Chaired by: TBC</span></b>	
10.15 - 10.45	<b>Discovering Compounds and Designing Materials</b> Prof. Ram Seshadri
10.45 – 11.15	<b>Single-crystal perovskite heterostructures</b> Prof. Hemamala Karunadasa
11.15 – 11.45	<b>Coffee Break</b>
11.45 – 12.15	<b>AI for molecular design, synthesis, and analysis</b> Prof. Connor Coley
12.15 – 12.45	<b>Autonomous research machines: Self-Optimising New Chemistry</b> Prof. Ruth Misener
12.45 – 14.00	<b>Lunch Break &amp; Poster Session</b>
<b>Session 2: <span style="float: right;">Chaired by: TBC</span></b>	
14.00 – 14.30	<b>Multimodal Design of Metal-Organic Frameworks</b> Prof. Aron Walsh
14.30 – 15.00	<b>Structural transitions in NaNiO<sub>2</sub> - A Model System for Ni-rich Battery Electrodes</b> Prof. Sian Dutton
15.00 – 15.30	<b>Coffee Break</b>
15.30 – 16.00	<b>Sustainable Materials Science for a Circular Economy</b> Prof. Anke Weidenkaff
16.00 – 16.30	<b>Strategies to design quantum materials with exotic properties</b> Prof. Roser Valentí

**PROGRAMME: Wednesday 13<sup>th</sup> November 2024**

<b>Session 3:</b>		<b>Chaired by: TBC</b>
<b>09.00 - 10.00</b>	<b>Coffee</b>	
<b>10.00 – 10.30</b>	<b>Accelerating Chemical Discovery and Development with Machine Learning and Automation.</b> Prof. Klavs Jensen	
<b>10.30 – 11.00</b>	<b>Transforming Lab Automation with Intelligent Robotic Scientists</b> Dr. Gabriella Pizzuto	
<b>11.00 – 11.30</b>	<b>Coffee Break</b>	
<b>11.30 – 12.00</b>	<b>The Dutch BigChemistry consortium: towards a self-driving lab for complex molecular systems</b> Prof. Wilhelm Huck	
<b>12.00 – 12.30</b>	TBC	
<b>12.30 – 14.00</b>	<b>Lunch Break &amp; Poster Session</b>	
<b>Session 4:</b>		<b>Chaired by: TBC</b>
<b>14.00 – 14:30</b>	<b>Accelerated discovery through distribution and democratization of self-driving labs – A case study for batteries and electrocatalysts</b> Prof. Tejs Vegge	
<b>14.30 – 15.00</b>	<b>A Robotic AI-Chemist Integrating Theory and Practice</b> Prof. Jun Jiang	
<b>15.00 – 15.30</b>	<b>Coffee Break</b>	
<b>15.30 – 16.00</b>	<b>Explainable AI for justifying automated decisions in real world domains</b> Prof. Katie Atkinson	
<b>16.00 – 16.30</b>	<b>Surprise Talk – To be announced on the day!</b>	
<b>16.30 – 17.30</b>	<b>Networking Drinks &amp; Poster Presentation Session</b>	
<b>17.30 – 18:30</b>	<b>Anfield Stadium Tours (pre booked) &amp; Networking Drinks &amp; poster Session Continued</b>	
<b>19:00 – 22:00</b>	<b>Conference dinner 18:45 for seating at 19:00 in The Chemistry Suite, 3<sup>rd</sup> Floor, Main Stand, Anfield Stadium</b>	

PROGRAMME: Thursday 14<sup>th</sup> November 2024

Session 5:		Chaired by: TBC
09.30 - 10.00	Coffee	
10.00 – 10.30	<b>Supramolecular polymer material design on multiple length scales</b> Prof. Emily Draper	
10.30 – 11.00	<b>Multi-fidelity Bayesian optimization of nanoporous materials for Xe/Kr separations</b> Prof. Cory Simon	
11.00 – 11.30	Coffee Break	
11.30 – 12.00	<b>Towards Electrochemical Solutions for Hydrogen Production, Storage, and Delivery</b> Prof. Sossina Haile	
12.00 – 12.30	<b>Data-Driven Innovation in Broadband Emitting Layered Nanomaterials</b> Prof. Milena Arciniegas	
12.30 – 14.00	Lunch Break	
Session 6:		Chaired by: TBC
14.00 – 14:30	<b>How can machine learning guided experimentation advance functional materials research...and how might it hinder us?</b> Prof. Joshua Schrier	
14.30 – 15.00	<b>I, for one, welcome our new AI partners</b> Dr. Ian Foster	
15.00 – 15.30	<b>Understanding and controlling the crystallisation dynamics of halide perovskites: The path to improved performance and stability</b> Prof. Nakita Noel	
15.30 – 16:00	Prize Presentation & Closing remarks	