

## DAY ONE – Tuesday 12<sup>th</sup> November 2024

09.00 – 10.00

**Registration and Coffee**

10.00 – 10.15

**Welcome & Intro to the LRC**

Prof. Andrew I Cooper

*Director, Leverhulme Research Centre for Functional Materials Design*

### Session 1: Chaired by Dr. Lauren McHugh

10.15 - 10.45

**Discovering Compounds and Designing Materials**

Prof. Ram Seshadri

*University of California*

10.45 – 11.15

**Single-crystal perovskite heterostructures**

Prof. Hemamala Karunadasa

*Stanford University*

11.15 – 11.45

**Coffee Break**

11.45 – 12.15

**AI for molecular design and synthesis**

Prof. Connor Coley

*Massachusetts Institute of Technology*

12.15 – 12.45

**Autonomous research machines: Self-Optimising New Chemistry**

Prof. Ruth Misener

*Imperial College London*

12.45 – 14.00

**Lunch Break & Poster Session**

### Session 2: Chaired by Dr. Linjiang Chen

14.00 – 14.30

**Multimodal Design of Metal-Organic Frameworks**

Prof. Aron Walsh

*Imperial College London*

14.30 – 15.00

**Structural transitions in NaNiO<sub>2</sub> - A Model System for Ni-rich Battery Electrodes**

Prof. Sian Dutton

*University of Cambridge*

15.00 – 15.30

**Coffee Break**

15.30 – 16.00

**A 'cobotic' automation strategy for handling pyrophoric, explosive and unstable compounds**

Dr. Nicola Bell

*University of Glasgow*

16.00 – 16.30

**Strategies to design quantum materials with exotic properties**

Prof. Roser Valentí

*Goethe University Frankfurt*

## DAY TWO – Wednesday 13<sup>th</sup> November 2024

### Session 3: Chaired by Dr. Jean-Francois Ayme

- 09.00 - 10.00**      **Coffee & Breakfast**
- 10.00 – 10.30**      **Accelerating Chemical Discovery and Development with Machine Learning and Automation**  
Prof. Klavs Jensen  
*Massachusetts Institute of Technology*
- 10.30 – 11.00**      **Transforming Lab Automation with Intelligent Robotic Scientists**  
Dr. Gabriella Pizzuto  
*University of Liverpool*
- 11.00 – 11.30**      **Coffee Break**
- 11.30 – 12.00**      **The Dutch BigChemistry consortium: towards a self-driving lab for complex molecular systems**  
Prof. Wilhelm Huck  
*Radboud University Nijmegen*
- 12.00 – 12.30**      **Data-Driven Innovation in Broadband Emitting Layered Nanomaterials**  
Prof. Milena Arciniegas  
*Italian Institute of Technology*
- 12.30 – 14.00**      **Lunch Break & Poster Session**

### Session 4: Chaired by Dr. Victoria Berryman

- 14.00 – 14:30**      **Accelerated discovery through distribution and democratization of self-driving labs – A case study for batteries and electrocatalysts**  
Prof. Tejs Vegge  
*Technical University of Denmark*
- 14.30 – 15.00**      **A Robotic AI-Chemist Integrating Theory and Practice**  
Prof. Jun Jiang  
*University of Science and Technology of China*
- 15.00 – 15.30**      **Coffee Break**
- 15.30 – 16.00**      **Explainable AI for justifying automated decisions in real world domains**  
Prof. Katie Atkinson  
*University of Liverpool*
- 16.00 – 16.30**      **Surprise Talk – To be announced on the day!**
- 16.30 – 17.45**      **Networking Drinks & Poster Presentation Session**
- 17.45 – 18:45**      **Anfield Stadium Tours (pre booked), Networking Drinks & Poster Presentation Session**
- 19:00 – 22:00**      **Conference dinner 18:45 for seating at 19:00 in The Chemistry Suite, Main Stand, Anfield Stadium**

## DAY THREE – Thursday 14<sup>th</sup> November 2024

### Session 5: Chaired by Dr. Charlotte Boot

09.00 - 10.00 **Coffee & Breakfast**

10.00 – 10.30 **Supramolecular polymer material design on multiple length scales**  
Prof. Emily Draper  
*University of Glasgow*

10.30 – 11.00 **Multi-fidelity Bayesian optimization of nanoporous materials for Xe/Kr separations**  
Prof. Cory Simon  
*Oregon State University*

11.00 – 11.30 **Coffee Break**

11.30 – 12.00 **Towards Electrochemical Solutions for Hydrogen Production, Storage, and Delivery**  
Prof. Sossina Haile  
*Northwestern University*

12.00 – 12.30 **How can machine learning guided experimentation advance functional materials research...and how might it hinder us?**  
Prof. Joshua Schrier  
*Fordham University*

12.30 – 14.00 **Lunch Break**

### Session 6: Chaired by Dr. Robert Woodward

14.00 – 14:30 **Sustainable Materials Science for a Circular Economy**  
Prof. Anke Weidenkaff  
*Technical University of Darmstadt*

14.30 – 15.00 **Title: Human-algorithm collaborative Bayesian optimization for chemical processes**  
Dr. Antonio del Rio Chanona  
*Imperial College London*

15.00 – 15.30 **Understanding and controlling the crystallisation dynamics of halide perovskites: The path to improved performance and stability**  
Prof. Nakita Noel  
*University of Oxford*

15.30 – 16:00 **Prize Presentation & Closing remarks**