Wednesday 8 July

09.30	**Registration and refreshments**
10-10.20	James Kermode, Defining Best Practice for Generative AI in Doctoral Study
10.20-10.35	**Cohort 7 (year 1) project overviews** **Chair: Nick Hine**
	Lucas Belz-Koeling, Machine learning of energy barriers for reaction network discovery of drug-like molecules
	Archie Brew, Development of DFT methods to study atomic structure and pressure effects in f- electron materials
	Peter Noordman, PhonIon: Modelling ultrafast THz pump-X-ray probe spectroscopies for ion dynamics in batteries
10.35-11.05	**Cohort 5 (year 3) presentation** **Chair: Ben Gosling (alumni)**
	Nojus Plungė, Deep energy modelling of phase-field fracture
11.05-11.30	**Refreshment break**
11.30-12.15	**Cohort 6 (year 2) presentations** **Chair: Geraldine Anis (alumna)**
	Keyi Wei, Structural and Mechanistic Insights into Gram-Negative Bacterial Pathways
	Facundo Costa, Data Driven Alpha Titanium Dislocation Glide
	George Simmons, Physics Informed Priors for Machine Learning Interatomic Potentials
12.15-13.30	**Lunch**
13.30-16.30	HetSys External Advisory Board (invited members only)
14.00 onwards	Team building event (all cohorts and alumnus), Courtyard at Scarman)
17.00	**Barbeque, Scarman outdoor area**

Thursday 9 July

09.30	**Registration and refreshments**
10.00-10.15	**Cohort 7 (year 1) project overviews** **Chair: Livia Bartók-Pártay**
	Jasper Allen, A picture worth a thousand atoms: 2D image to 3D nanostructure mapping by merging simulated and measured data
	Tristan McCarthy, Atomic-Level Defect Characterisation via Data Fusion: Integrating Ptychography, EELS & 1st Principles Calculations
	Sindi Semanaj, AMPLIFY: Advancing Membrane Protein Learning for Improved Factorial Yield
10.15-11.15	**Cohort 5 (year 3) presentations** **Chair: Ziad Fakhoury (alumni)**
	Matthew Christensen, Quantum Algorithms for Plasma and Fusion Physics
	Yuji Go, Modelling transport phenomena in complex electronic structures
11.15	Group photograph, WBS steps (ALL)
11.35	**Refreshment break**
12.00-13.00	**KEYNOTE: Professor Timm Krüger** **Chair: Radu Cimpeanu** **Computer Simulations in Science and Engineering - What Can We Learn, and How Can They Help Us?** Fluid and Suspension Dynamics, University of Edinburgh
13.00-14.15	**Lunch**
14.15-15.00	**Cohort 6 (year 2) presentations** **Chair: Vincent Fletcher (Cohort 4, year 4)**
	Luca Gasparro, Computing the Glass Transition Temperature of Hydrophobic and Hydrophilic Painkillers via Molecular Dynamics Simulations
	Sean Wu, Towards Correlative 4D-STEM Ptychography and EELS for Cryogenic Single-Particle Analysis
	Swathi Mahashetti, Modelling Point Defects and their properties in Perovskite bulks, surfaces and interfaces

15.00-15.30 **Cohort 5 (year 3) presentations**
Chair: Adam Fisher (alumni)

Valdas Vitartas, Uncertainty-Aware Machine Learning Hamiltonians with On-Demand SCF Refinement

15.30-16.00 **Refreshment break (if you are presenting a poster or bringing an object, please go to the Lakeside suite now to set up)**

16.00-17.00 **Cohort 5 (year 3) presentations**
Chair: Hubert Naguezewski (Cohort 4, year 4)

YC Wong, Are we getting very close to good long range machine learning models?

Philip Jones, What's that made of? Modelling muonic X-ray radiation for quantitative elemental analysis

17.00-17.30 **Cohort 6 (year 2) presentations:**
Chair: Chris Woodgate (alumni)

George McKay, Error bounds in weakly symmetric quantum trajectories

Luca Seaford, Learning Grand-Canonical Free-Energy Surfaces for Au Electrodeposition on Graphene Bilayers

17.30 **Drinks reception in Lakeview Suite**
Posters, 3d models and objects

19.00 **Conference Dinner, Courtyard suite**

Friday 10 July

09.30	**Registration and refreshments**
10.00	**Cohort 7 (year 1) presentation overviews** **Chair: James Kermode**
	Anton Oleinik, Modelling interfacial flows in porous media: a hybrid asymptotic-computational approach
	Kunlin Cai, Physics-informed machine learning-based swelling models for future battery cells
	Stephan Gambart, Programmable fluids: Continuum models for designing multi-stable meta-fluids
10.15-11.15	**Keynote: Professor Birgit Strodel** **Chair: Livia Bartók-Pártay** **Peptides Under the Microscope: From Amyloid Aggregation Mechanics to Computational Design** Institute of Biological Information Processing (IBI-7: Structural Biochemistry), Research Centre Jülich, Germany Computational Biochemistry, Heinrich Heine University Düsseldorf, Germany
11.15-11.30	**Refreshment break**
11.30-12.30	**Cohort 5 (year 3) presentations** **Chair: Tom Rocke (alumni)**
	Zahra Bhatti, Modeling excited states for the simulation of UV/Vis spectra
	Roman Shantsila, From Automation to Application: Machine-Learned Potentials for Building and Modelling Battery Interfaces
12.30-13.45	**Lunch**
13.45-14.30	**Cohort 6 (year 2) presentations** **Chair: Seb Dooley (Cohort 4, year 4)**
	David Bewicke, Simulating Exoplanet Magnetospheres
	Maks Diakiewicz, Modelling supercooling dynamics of phase change materials
	Rumesh Sudhaharan, On thin ice: modelling and simulation of an unstable interface
14.30	**Closing remarks and prizes** **Livia Bartók-Pártay and Mike Ward, Vice Provost and Chair of the Faculty of Science, Engineering and Medicine**
14:40	Conference close