Tuesday 10 September

11:00	Registration and refreshments
12:00	Lunch
12:45	**Welcome and introductions** Volker Deringer & Fernanda Duarte, Co-*chairs of Scientific Committee*
12:55	**Outline of Discussion format** Emma Gorrell & Lauren Yarrow-Wright, *Royal Society of Chemistry*
13:30	**Introductory lecture – Spiers memorial lecture** (Session chair: Volker Deringer) Alán Aspuru-Guzik *University of Toronto, Canada*
14:30	Short break (no refreshments)
	Session 1: Discovering chemical structure (Session chair: Graeme Day)
14:45	**Beyond theory-driven discovery: introducing hot random search and datum-derived structures** Chris Pickard *University of Cambridge, UK*
14:50	**Integration of generative machine learning with the heuristic crystal structure prediction code FUSE** Chris Collins *University of Liverpool, UK*
14:55	**Large property models: a new generative machine-learning formulation for molecules** Brett Savoie *Purdue University, USA*
15:00	Discussion
16:15	Refreshments
	Session 1 continued: Discovering chemical structure (Session chair: Janine George)
16:45	**Data-efficient fine-tuning of foundational models for first-principles quality sublimation enthalpies** Venkat Kapil *University of Cambridge, UK*
16:50	**Knowledge distillation of neural network potential for molecular crystals** Takuya Taniguchi *Waseda University, Japan*
16:55	**Modelling ligand exchange in metal complexes with machine learning potentials** Veronika Jurásková *University of Oxford, UK*
17:00	Discussion
18:15	Poster session and wine reception
19:45	Close

Wednesday 11 September

	Session 2: Discovering structure–property correlations (Session chair: Nadine Schneider)
09:00	**Web-BO: towards increased accessibility of Bayesian optimisation (BO) for chemistry** Kim Jelfs *Imperial College London, UK*
09:05	**Sequence determinants of protein phase separation and recognition by protein phase-separated condensates through molecular dynamics and active learning** Arya Changiarath Sivadasan *Johannes Gutenberg University of Mainz, Germany*
09:10	**Discovery of highly anisotropic dielectric crystals with equivariant graph neural networks** Yuchen Lou, Alex Ganose *Imperial College London, UK*
09:15	Discussion
10:30	Refreshments
	Session 2 continued: Discovering structure–property correlations (Session chair: Fernanda Duarte)
11:00	**Leveraging natural language processing to curate the tmCAT, tmPHOTO, tmBIO, and tmSCO datasets of functional transition metal complexes** Heather Kulik *Massachusetts Institute of Technology, USA*
11:05	**Are we fitting data or noise? Analysing the predictive power of commonly used datasets in drug-, materials-, and molecular-discovery** Daniel Crusius *University of Oxford, UK*
11:10	**Prediction rigidities for data-driven chemistry** Sanggyu Chong *EPFL, Switzerland*
11:15	**Accurate and reliable thermochemistry by data analysis of complex thermochemical networks using active thermochemical tables: the case of glycine thermochemistry** Branko Ruscic *Argonne National Laboratory, USA*
11:20	Discussion
13:00	Lunch
	Session 3: Discovering trends in big data (Session chair: Philippe Schwaller)
13:45	**Specialising and analysing instruction-tuned and byte-level language models for organic reaction prediction** Jiayun Pang *University of Greenwich, UK*
13:50	**Predictive crystallography at scale: mapping, validating, and learning from 1000 crystal energy landscapes** Christopher Taylor *University of Southampton, UK*
13:55	**Optical materials discovery and design with federated databases and machine learning** Matthew Evans *UCLouvain, Belgium*
14:00	Discussion
15:15	Refreshments
	Session 3 continued: Discovering trends in big data (Session chair: Janine George)
15:45	**How big is big data?** Claudia Draxl

	Humboldt-Universität zu Berlin, Germany
15:50	**Making the InChI FAIR and sustainable while moving to inorganics** Gerd Blanke *RWTH Aachen University, Germany*
15:55	Discussion
16:45	**Panel Discussion - EDI in Digital Chemistry** Panel members: Alán Aspuru-Guzik, *University of Toronto, Canada* Stephen Hendry, *Royal Society of Chemistry* Kim Jelfs, *Imperial College London, UK* Chaired by Volker Deringer & Fernanda Duarte
17:30	Poster session and wine reception
19:00	Close
19:30	Conference dinner

Thursday 12 September

	Session 4: Discovering synthesis targets (Session chair: Philippe Schwaller)
09:00	**Analysis of uncertainty of neural fingerprint-based models** Miriam Mathea *BASF, Germany*
09:05	**Re-evaluating retrosynthesis algorithms with Syntheseus** Marwin Segler *Microsoft Research AI for Science, UK*
09:10	**Embedding human knowledge in material screening pipeline as filters to identify novel synthesizable inorganic materials** Basita Das *Massachusetts Institute of Technology, USA*
09:15	Discussion
10:30	Refreshments
	Session 4 continued: Discovering synthesis targets (Session chair: Volker Deringer)
11:00	**Mapping inorganic crystal chemical space** Aron Walsh *Imperial College London, UK*
11:05	**A critical reflection on attempts to machine-learn materials synthesis insights from text-mined literature recipes** Wenhao Sun *University of Michigan, Ann Arbor, USA*
11:10	Discussion
12:00	**Concluding remarks lecture** (Session chair: Fernanda Duarte) Andy Cooper *University of Liverpool, UK*
12:30	**Acknowledgements** Volker Deringer & Fernanda Duarte, Co-*chairs of Scientific Committee*
12:45	Close of meeting and lunch