MLCM-24 schedule
mlcm-24.github.io   [updated 05/05/24]

Time	5/20 MONDAY	5/21 TUESDAY	5/22 WEDNESDAY	5/23 THURSDAY
8:45 - 9:00 AM	Marianne Francois *T-division, LANL* — opening remarks			
9:00 - 9:30 AM	*plenary* Anatole von Lilienfeld *University Of Toronto / Vector Institute* — Quantum Machine Learning	*plenary* Gabor Csanyi *University of Cambridge* — Foundation models for materials chemistry	*plenary* Alexandre Tkatchenko *University of Luxembourg* — Navigating Chemical Compound Space with Machine Learning	*plenary* Markus Reiher *ETH Zurich* — Lifelong Machine Learning Potentials
9:30 - 10:00 AM	*plenary* Oleg Prezhdo *University of Southern California* — Nonadiabatic Molecular Dynamics with Machine Learning	*plenary* Mario Barbatti *Aix Marseille University, CNRS, ICR* — Machine Learning Nonadiabatic Dynamics	*plenary* Roberto Car *Princeton University* — Deep potential models for equilibrium and near equilibrium processes	*plenary* Olexandr Isayev *Carnegie Mellon University* — AIMNet2: Robust neural network potential for organic, element-organic molecules and chemical reactions
10:00 - 10:20 AM	David Balcells *University of Oslo* — Generative Machine Learning for Transition Metal Chemistry	Reinhard Maurer *University of Warwick* — Machine learning of electronic structure for molecular design	Nong Artrith *Debye Institute for Nanomaterials Science* — ML & XAS for Amorphous Materials	Johannes Margraf *University of Bayreuth* — Materials Discovery with Foundation Models
10:20 - 10:40 AM	Volker Deringer *University of Oxford* — Data-driven interatomic potentials for inorganic materials chemistry	Karel Berka *Palacky University Olomouc* — MolMeDB - free database of molecules on membranes	Matthias Rupp *Luxembourg Institute of Science and Technology (LIST)* — Thermal transport via machine-learning potentials	Zsuzsanna Koczor-Benda *University of Warwick* — Machine learning-based molecular design for plasmonic nanosystems
10:40 - 11:00 AM	Eva Zurek *University at Buffalo, SUNY* — Machine Learned Interatomic Potentials for Binary Carbides Trained on the AFLOW Database	Alexander Shapeev *Skolkovo Institute of Science and Technology* — From quantum mechanics to phase diagrams with machine learning	*interactive session* Jason Hattrick-Simpers *University of Toronto* — Tutorial on the use of LLMs in Science	Tom Penfold *Newcastle Univeristy* — Deep Neural Networks for X-ray Spectroscopy: Hero or Zero?
11:00 - 11:20 AM	Rohit Goswami *University of Iceland / Quansight Labs* — Throwaway Gaussian Processes for Saddle Searches	Julien Lam *CNRS* — Exploiting constrained linear models for machine-learning interaction potentials		Aurora Clark *University of Utah* — ML in Chemical Separations - Connecting Reaction Stoichiometry with Solution Structure
11:20 - 11:40 AM	Matthew Carbone *Brookhaven National Laboratory* — TBD	Dmitry Zubarev *IBM Research* — Foundational Models for Chemical Discovery		Connor Coley *MIT* — Molecular design and the intersection with synthesis
11:40 am - 1:00 PM	LUNCH BREAK			
1:00 - 1:30 PM	*plenary* Richard Hennig *University of Florida* — Accelerating Materials Discovery Through Deep Learning and Ultra-Fast Potentials	*plenary* Kieron Burke *University of California, Irvine* — Machine Learning Density Functionals	*plenary* Alan Aspuru-Guzik *University of Toronto* — TBA	*plenary* Rebecca Lindsey *University of Michigan, Ann Arbor* — Explaining Performance of Physics-Informed Machine-Learned Interatomic Models
1:30 - 1:50 PM	Wissam Saidi *NETL* — Materials Modeling and Machine Learning	Y Z *University of Michigan* — Unusual Dynamics of Tetrahedral Liquids Caused by the Competition between Dynamic Heterogeneity and Structural Heterogeneity	Pavlo Dral *Xiamen University* — From fast potentials for dynamics to learning dynamics	Noa Marom *Carnegie Mellon University* — Applications of Machine Learning in First Principles Materials Simulations
1:50 - 2:10 PM	Avanish Mishra *LANL* — Learning from 'Small' Data Using Physics-Based Descriptors	Joshua Rackers *Genentech / Prescient Design* — Building Physics into AI for Drug Discovery	Aditya Nandy *UCLA / University of Chicago* — Leveraging Community Knowledge to Forge a Path Forward for Transition Metal Complex and Metal-Organic Framework Design	Marivi Fernandez-Serra *Stony Brook University* — Learning the exchange and correlation functional in DFT
2:10 - 2:30PM	Fang Liu *Emory University* — Machine learning aided chemical discovery in the solution phase	Arthur Mar *University of Alberta* — Discovery of Inorganic Solids with Desired Structure Motifs Guided by Machine Learning	Richard Messerly *LANL* — Nanoreactor active learning: Discovering chemistry with a general reactive machine learning potential	David Yaron *Carnegie Mellon University* — Quantum chemical Hamiltonians as flexible and interpretable model forms for machine learning
2:30 - 2:50 PM	Chenru Duan *Microsoft* — Diffusion models on sampling rare events in chemistry	Sakib Matin *LANL* — Machine Learning Potentials with long-range Coulomb interaction: Atomistic simulations of water	Ankur Chaterjee *Nicolaus Copernicus University* — Spatio-temporal dependancies of in-plane and cross-plane thermal transport proerties by hybrid architecture of CNN and RNN	Jenna Pope *Pacific Northwest National Laboratory* — Accelerating Atomic-scale Simulations of Molecules and Materials with Neural Network Potentials
2:50 - 3:10 PM	Rose Cersonsky *University of Wisconsin-Madison* — Data-driven approaches to chemical and materials science:the impact of data selection, representation, and interpretability	Chiho Kim *GATech / Matmerize, Inc.* — Machine Learning-Aided Design of Biodegradable Polymers	Bakhtiyor Rasulev *North Dakota State University* — Application of Mixture-type Descriptors in Machine Learning Modeling of Materials	Vignesh Kumar *Nicolaus Copernicus University* — The critical role of XC potential in DFT: Our Big data analysis into DFT
3:10 - 3:30 PM	Johannes Hachmann *University at Buffalo* — TBA	Marina Meila *University of Washington* — TBA	Emily Shinkle *LANL* — Thermodynamic Transferability in Coarse-Grained Force Fields using Graph Neural Networks	Puck van Gerwen *EPFL* — EquiReact: Equivariant Neural Networks for Chemical Reactions
3:30 - 3:50 PM	Will Bricker *University of New Mexico* — Machine-learned electron densities of nucleic acids	Daniel Schwalbe-Koda *UCLA* — Unifying Views on the Extrapolation Power of Machine Learning Potentials and Materials Thermodynamics	Maria Chan *Argonne National Laboratory* — Theory-informed ML for Microscopy, Spectroscopy, and Scattering	Jing Huang *Westlake University* — DP/MM: a hybrid force field model for zinc-protein dynamics