

MLCM-24 schedule

mlcm-24.github.io

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