MLCM-24 schedule

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

	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	**Maria Chan** *Argonne National Laboratory* Theory-informed ML for Microscopy, Spectroscopy, and Scattering	**Daniel Schwalbe-Koda** *UCLA* Unifying Views on the Extrapolation Power of Machine Learning Potentials and Materials Thermodynamics	**Jing Huang** Westlake University DP/MM: a hybrid force field model for zinc-protein dynamics