Table of contents

Young Researchers' Workshop on Machine Learning for Materials | (smr 3701)

Wednesday 11 May 2022

notitle - (09:00-18:00)

time	title	presenter
09:00	Data-manifold Characterisation: Estimating Intrinsic Dimension, Density, and Density Peaks with DADApy	ALDO GLIELMO
10:20	Coffee Break	
11:00	Training Neural Network Potentials with PANNA	FRANCO PELLEGRINI
12:20	Lunch Break & Registrations	
13:40	Opening Remarks	
14:00	Symmetry and Uncertainty-aware Models of Interatomic Interactions for Fast Molecular Dynamics	BORIS KOZINSKY
14:40	A Unified Understanding of Equivariant Interatomic Potentials	ILYES BATATIA
15:00	Atomic Cluster Expansion based Force Fields for Molecular Materials	DAVID PETER KOVACS
15:20	Coffee Break	
15:40	Unsupervised Learning of Group Invariant and Equivariant Representations and its Application to Molecular Conformations	ROBIN WINTER
16:00	Unsupervised Representation Learning on Molecular Conformations	TUAN LE
16:20	Interpretable Embeddings from Molecular Simulations using Gaussian Mixture Variational Autoencoders	YASEMIN BOZKURT VAROLGÜNES
16:40	Learning Explainable Models from Complex Data with Applications in QSAR (Quantitative Structure-activity Relationships) Modelling	SASO DZEROSKY
17:20	Transportation to SISSA	