

**Program: NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights
Kiel, Germany, September 17-21, 2023**

TIME	Sunday, Sep 17, 2023	TIME	Monday, Sep 18, 2023	Tuesday, Sep 19, 2023	TIME	Wednesday, Sep 20, 2023	Thursday, Sep 21, 2023
		8:00			8:00		Kiel arrival 8:00
		9:00			9:00	Crystal growth and other things: Introduction to the session by the chair: Tom Purcell	deboarding
		9:15	Artificial Intelligence: Introduction to the session by the chair: Wahib Aggoune		9:15	Hong Jiang: Combining cluster expansion and machine learning force field for configurationally disordered materials	
		9:30	Runhai Ouyang: Development of the SISSO methods for Symbolic Regression in Materials Science		10:00	Yuan Yuan Zhou: Grand-canonical replica exchange approach: several potential application examples	
		10:15	Tom Purcell: Recent advances in the SISSO method and their implementation in the SISSO++ code	Oslo Excursion, Discussion & Preparation of the Next Sessions in Small Groups 9:00 - 15:00	10:30	Break	
		10:45	Break		10:30	Qaem Hassanzada: Kinetic Monte Carlo Approach for Molecular Beam Epitaxy Growth of Crystals	
		11:00	Yi Yao: Performance Boosting Portable Acceleration of SISSO++ for Symbolic Descriptor Learning		10:45		
		11:30	Lucas Foppa: Beyond a Single Description in Subgroup Discovery of Exceptional Materials: Coherent Collections of Rules Clustered By Similarity		11:15	Evgeny Moerman: Affordable and highly accurate coupled-cluster band gaps in the thermodynamic limit	
					11:30	Copenhagen arrival 12:00	
13:00	Check in 13:00-14:00	12:00	Lunch	Lunch	12:00	Lunch	
14:00							
		14:00	Kisung Kang: Active-Learning Methodology for Interatomic Potentials in Large-Scale Molecular Dynamics		14:00		
		14:30	Daniel Speckhard: Extrapolation of DFT results to the complete basis set limit		14:30		
		15:00	Shuo Zhao: Anisotropic thermal conductivity from ab initio Green-Kubo		15:00		
		15:30	Luigi Sbailo: Uncertainty quantification in deep neural networks to detect out-of-distribution samples		15:30		
		16:00	Break	Oslo departure 16:00	16:00	Copenhagen Excursion, Discussion & Workshop Summary in Small Groups 12:00 - 18:00	
		16:15	FHI-aims: Introduction to the session by the chair: Mariana Rossi	Catalysis and other things: Introduction to the session by the chair: Lucas Foppa	16:15		
		16:30	Volker Blum: FHI-aims, ELSI, and some Adventures in Perovskites	Annabella Selloni: Molecular simulations of aqueous solutions and interfaces with machine learning potentials	16:30		
		17:15	Andrey Sobolev: Recent developments in GIMS	Herzain Isaac Rivera Arrieta: Multi-target screening of heterogeneous catalysts through the exceptional model mining approach	17:15		
		17:45	Min-Ye Zhang: GW method for periodic systems with numeric atom-centered orbitals	Akhil Sugathan Nair: Multi-fidelity modelling for materials discovery with sequential learning	17:45		
		18:15	Overview Oslo City	Wahib Aggoune: Designing new memristor materials	18:15		
18:15	Roberto Car: Machine Learning and Coarse Graining in Molecular Simulations	18:30		Overview Copenhagen City	18:45	Copenhagen departure 19:00	
19:00	Dinner	19:00	Dinner	Dinner	19:00	Dinner	
21:00	Aaron Kelly: Revealing Ultrafast Phonon-Mediated Inter-Valley Scattering through Transient Absorption and High Harmonic Generation Spectroscopies	21:00	Oslo Fjord 21:00		21:00	Mariana Rossi: Quantum Fluctuations in Weakly Bound Materials	
		21:15		Stefano Curtarolo: Disordered enthalpy-entropy descriptor for high-entropy ceramics discovery	21:15		
21:30		21:45			21:45	Overview Kiel City	
22:00		22:00			22:00		