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Conference on Frontiers in Atomistic Simulations: from Physics to Chemistry and Biology | (smr 4098)

Monday 08 September 2025

notitle - Budinich Lecture Hall (LB) (09:00-18:00)

time	title	presenter
09:00	ICTP Introduction	ALI HASSANALI
09:10	Four Generations of High-Dimensional Neural Network Potentials	JOERG BEHLER
09:40	TBA	PABLO PIAGGI
10:10	Towards unified representation learning and sampling	PRATYUSH TIWARY
10:40	Coffee break	
11:20	TBA	MICHELE CERIOTTI
11:50	TBA	LAURA GAGLIARDI
12:30	Lunch	
14:00	TBA	LUIGI BONATI
14:30	TBA	UMBERTO RAUCCI
15:00	Automatic Reaction Discovery by Biasing Deep-Learned Skewed Distributions	GIOVANNI MARIA PICCINI
15:30	Coffee break	
16:10	Data-efficient Deep Potential for Enhanced Sampling Simulations of Complex Systems	TARAK KARMAKAR
16:40	TBA	JAYASHRITA DEBNATH
17:10	TBA	ZHIPAN LIU
17:40	Buffer / Announcements	