

Training School: MOF Computational Tools and Machine Learning



October 14		
Time	Trainers	Focus (Lectures: 30 min talk+10 min Q&A)
10:00-10:20	Ilknur Erucar	Opening talk-overview of the program
10:20-11:00	Guillaume Maurin	ML force fields-based molecular simulations
11:00-11:20	Morning Coffee Break & Discussion Session	
11:20-12:00	Sven Rogge	MOFs under "pressure"
12:00-12:30	Seda Keskin	Panel Discussion: What is next? ML integrated materials informatics
12:30-13:10	Peyman Moghadam (Online)	Recent advances in MOF database development
13:10-14:15	Lunch Break	
14:15-14:30	Afternoon Coffee Break & Discussion Session	
14:30-15:10	George E. Froudakis	Gas Adsorption Meets Deep Learning
15:10-15:40	Aydin Ozcan	Panel Discussion: New advancements with data-driven and simulation approaches
15:40-16:20	Jack Evans (Online)	Enhanced sampling in the simulations for microporous materials
16:20-16:45	Quim Pena	Panel Discussion: MOFs & Biomedicine: hope, promise and expectations
16:50-17:30	Manuel Tsotsalas (Online)	Text mining and new techniques for MOF database search
October 15		
9:40-10:00	Quim Pena	Reimbursement Details
10:00-10:40	Student Discussion (Chair: Hakan Demir)	Student Panel, Hands-On-Session GCMC simulations, MOF Databases, Gas adsorption simulations
10:40-11:00	Morning Coffee Break & Discussion Session	
11:00-11:40	Rochus Schmid (Online)	Adsorption induced phase transformations simulated beyond PBC
11:40-12:40	Student Discussion	Student Panel, Hands-On-Session MD simulations, ML examples
11:40-12:40	Future Progress (Team Meeting)	Future plans
12:40-13:40	Lunch Break	
Notes:	The building is AB4. (Architecture Building at Ozyegin University, Cekmekoy, ISTANBUL) Room number is G25 . Dinner plan will be shared via email. Zoom link will be shared with the participants for the hybrid sessions.	