

DFT Methods for Matter under Extreme Conditions

Tuesday, February 22, 2022

Session 3 (9:00 AM - 11:50 AM)

time	[id] title	presenter
9:00 AM	[15] Data-driven and Physics-Informed Modeling of Matter under Extreme Conditions	CANGI, Attila
10:00 AM	[24] Hyperparameter optimization for automated DFT surrogate model creation	FIEDLER, Lenz
10:20 AM	Coffee break	
10:50 AM	[42] Ab initio and machine learning-based simulations of hydrogen in the Earth's core	YUAN, Liang
11:20 AM	[49] Learning the exchange-correlation functional from nature with fully differentiable density functional theory	KASIM, Muhammad