Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis XI

Thursday, 19 June 2025

Session 6: Semi-empirical Methods (11:00 - 12:00)

time	[id] title	presenter
11:00	[26] (Expert) Material Informatics @ Freudenberg	KUNKEL, Christian
11:20	[27] Combining DFTB and Structure-Mapping for the Prediction of Transition Paths in Deactivation of ZnO@Cu Catalysts	SAMTSEVYCH, Artem
11:40	[28] Hard Carbon Done Right: Swarm Intelligence Ensemble Generation to Realise Full Atomic Decorrelation	HOLLAND, Julian