Session Program

Jun 16 – 20, 2025

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

Session 6

Thu, June 19

11:00 AM

Session 6: Semi-empirical Methods

Session |
Location: Haus der bayerischen Landwirtschaft, Rieder Str. 70, 82211 Herrsching am Ammersee, Germany

11:00 – 11:20 AM **(Expert) Material Informatics @ Freudenberg**

Speaker
Christian Kunkel

11:20 – 11:40 AM

Combining DFTB and Structure-Mapping for the Prediction of Transition Paths in Deactivation of ZnO@Cu Catalysts

Speaker
Artem Samtsevych

11:40 AM – 12:00 PM

Hard Carbon Done Right: Swarm Intelligence Ensemble Generation to Realise Full Atomic Decorrelation

Speaker
Julian Holland

12:00 PM