Session Program

16–20 Jun 2025

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

Session 6

Thursday 19 June

11:00

Session 6: Semi-empirical Methods
Session |
Location: Haus der bayerischen Landwirtschaft, Rieder Str. 70, 82211 Herrsching am Ammersee, Germany

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

Speaker
Christian Kunkel

11:20–11:40

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

Speaker
Artem Samtsevych

11:40–12:00

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

Speaker
Julian Holland

12:00