

Session Program

22-26 Apr 2024

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

**Session VII: Theory of Heat and Charge
Transport**

Friday 26 April

09:40

Session VII: Theory of Heat and Charge Transport

Session | **Location:** Hotel Marena Wellness & Spa Turystyczna 1, 72-415 Międzywodzie, Poland

09:40–10:20

A Perspective on Classical Force-Fields in the (Hype-)Times of Machine Learned Potentials

Speaker

Prof. Rochus Schmid

10:20–10:40

Introduction to Phonon Polaritons and Permittivity Function Modelling

Speaker

Dr Elena Gelžinytė

10:40

11:00

Session VII: Theory of Heat and Charge Transport

Session | **Location:** Hotel Marena Wellness & Spa Turystyczna 1, 72-415 Międzywodzie, Poland

11:00–11:20

Defects and Polarons in Magnesiumoxide

Speaker

Mr Christoph Dähn

11:20–11:40

A ML Interatomic Potential for Polaron Hopping

Speaker

Dr Matteo Rinaldi

11:40–12:10

Mirroring the Future - How Zeiss Enables Smaller, More Powerful and Energy-Efficient Microchips

Speaker

Dr Georg Michelitsch

12:10