

MM 7: Invited talk Erhart

Time: Monday 15:00–15:30

Location: H43

Invited Talk

MM 7.1 Mon 15:00 H43

Thermodynamics and optical response of nanoscale systems from atomistic simulations — •PAUL ERHART¹, TUOMAS ROSSI¹, MAGNUS RAHM¹, and MIKAEL KUISMA² — ¹Chalmers University of Technology, Department of Physics — ²University of Jyväskylä, Department of Chemistry

The properties of nanoparticles are sensitive to size, shape, composition, and environment, providing ample opportunities for material optimization and targeted design of functionalities. Here, I will summarize recent work from my group that addresses thermodynamic and optical properties of metallic nanoparticles.

Atomic scale simulations reveal an energy landscape as a function of size and shape that is more intricate than previously suggested. The

thus obtained particle type distributions demonstrate that the transition from icosahedral particles to decahedral and further into truncated octahedral particles occurs only very gradually, which has implications for the interpretation of experimental data.

Metal nanoparticles can also support localized surface plasmon resonances, which can decay into high-energy electrons and holes allowing hot-carrier generation for, e.g., photocatalysis. In this context, I will show ongoing work in which we follow plasmon formation as a collective excitation, track its subsequent decay into incoherent electron-hole transitions, and finally, obtain the corresponding hot-carrier distributions. Our work paves the way for addressing the spatiotemporal dynamics of hot-carrier generation in catalytically-relevant edge and corner sites of nanoparticles.