O 103: Invited Talk (Karsten Reuter)

Time: Friday 13:15–14:00 Location: TRE Phy

Invited Talk O 103.1 Fri 13:15 TRE Phy

Beat the heat! First-principles based modeling of micro- and macroscopic heat dissipation in heterogeneous catalysis

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First-principles electronic structure theory calculations are the indispensable basis for a predictive-quality modeling of catalytic activity. For a more comprehensive understanding of the catalytic function this basis needs to be linked to more coarse-grained approaches. First-principles kinetic Monte Carlo (kMC) simulations represent such an approach, which allows following the full system dynamics from picoseconds up to seconds, while fully accounting for the correlations, fluctuations and spatial distributions of the chemicals at the catalyst surface. A major challenge to the approach comes from the energy released in the exothermic surface reactions. I will sketch our recent efforts to augment the kMC simulations with an appropriate account of energy dissipation both at the atomistic and continuum level [1].

[1] S. Matera and K. Reuter, Catalysis Letters, 2009, 133, 156.