Eugene Wigner Colloquium

joint event of GRK 1558 and SFB 910

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"Towards *ab initio* modelling of heterogeneous catalysis: beyond the static, monostructure description"

One of the challenges of present and near future conversion, storage, and transportation of energy is its catalytic transformation into fuels. The widespread description and modelling of heterogeneous catalysis focus on energies and energy barriers, however the dynamics and statistical mechanics are also important. By focusing on gas-phase metal and metal-oxide (sub)nano clusters in a reactive atmosphere, I show how the accurate (and validated) knowledge of the (*ab initio*) potential energy surface cluster + reactant systems can be bridged to simple thermodynamic considerations for modeling the prediction of (meta)stable structures and compositions of the systems at realistic environmental conditions (finite temperature and pressure of the reacting atmosphere).

One of the most delicate assumptions of such model is that the configurational entropy is approximated by the harmonic vibrational entropy. This assumption is not always justified. In fact some (but not all) (sub)nano cluster systems exhibit even at moderate temperatures anharmonic behavior associated with the coexistence of a multiplicity of structures: fluxionality and liquid-like behavior. I show how massively parallelized (*ab initio*) replica exchange molecular dynamics and efficient reweighting techniques offer a way to describe the relative population of such higly-anharmonic systems, seamlessly bridging the vibrational to the configurational-change time scales.

In the last part, I show how, via carefully tailored statistical learning, *ab initio* data can be used for building physically meaningful models for estimating the properties of a given material.

GRK1558
research training group

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