O 110: New Methods: Theory

Time: Friday 10:30–10:45 Location: MA 005

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Error propagation in first principles kinetic Monte Carlo models — Sandra Döpking and •Sebastian Matera — Institut f. Mathematik, Freie Universität Berlin

The last years have seen an increasing interest in (chemical) kinetic models which have been parametrized using first principles electronic structure calculations. While these allow to access material properties without fitting the model to experimental data, commonly employed electronic structure theories rely on some approximations and thereby the estimated parameters carry an usually sizeable error. Using a first principles kinetic Monte Carlo model for the CO oxidation on the $RuO_2(110)$ surface as a example, we will address the propagation of these errors to the kinetic model's output. For this, we will employ a newly developed distribution based approach to global sensitivity analysis. This approach allows to estimate all sensitivity indices from a single set of sampling points of the parameter space and is also applicable to stochastic model outputs. Further, the resulting sensitivity indices might be interpreted as induced uncertainty by the respective uncertain parameter. For the model at hand, we find sizeable uncertainties but also that only a subset of all errors control this. Such information might be used to identify those parameters which are worth a determination with a more accurate electronic structure method or for identifying suitable descriptors for materials screening.