First-Principles Kinetic Monte Carlo for Surface Catalysis: From Exploratory Tool to Commodity

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First-principles based microkinetic modeling has evolved into a widely used approach in catalysis research. It combines the predictive-quality description of individual elementary processes with an account of their mesoscopic statistical interplay to yield measurable observables like catalytic activity or surface composition. Replacing mean-field rate equation based modeling, first-principles kinetic Monte Carlo (1p-kMC) thereby fully resolves the spatial distributions, correlations and fluctuations of the surface adlayer. In my talk I will illustrate current capabilities and frontiers of this approach, focusing among others on the hierarchical integration of 1p-kMC into continuum-level fluid dynamical simulations to account for heat and mass transfer effects in a macroscopic reactor, or on extensions to multi-lattice 1p-kMC to capture surface morphological transformations.