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# First-Principles Kinetic Monte Carlo Simulations: Concepts, Status and Frontiers

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Abstract:

First-principles microkinetic simulations have become standard tools in research on surface catalysis and many other areas [1,2]. They combine the predictive power of first-principles density-functional theory calculations with the possibility to treat extended time scales and larger ensembles of active sites. The lecture will survey the methodological foundations, as well as ongoing developments in the field.

[1] "First-Principles Kinetic Modeling in Heterogeneous Catalysis: An Industrial Perspective on Best-Practice, Gaps and Needs", M.K. Sabbe, M.-F. Reyniers, and K. Reuter, Catal. Sci. Technol. 2, 2010 (2012).
[2] "Ab Initio Thermodynamics and First-Principles Microkinetics for Surface Catalysis", K. Reuter, Catal. Lett. 146, 541 (2016).