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$dP_i(t)dt = - \sum_j k_{ij}P_i(t) + \sum_j k_{ji}P_j(t)$. (1) From a mathematical standpoint, Equation (1) is a system of coupled differential rate equations. Seemingly simple, it unfortunately becomes quickly unfeasible to solve explicitly for the number of possible states typically involved in surface catalysis (or diffusion or growth).

A Practical Guide to Surface Kinetic Monte Carlo Simulations

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