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A Practical Guide to Kinetic Monte Carlo Simulations and ...

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$dP_i(t)dt = \sum_j k_{ij}P_j(t) - k_{ji}P_i(t)$ . (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

The guidelines of this textbook are numerous example programs, flux diagrams, schemes, and figures presenting the obtained results. Step by step, the authors explain how steady state Monte Carlo Simulation (MCS) and time resolved, so-called kinetic or dynamic Monte Carlo Simulation (KMCS), schemes, respectively, can be set up.

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Abstract: This review article is intended as a practical guide for newcomers to the field of kinetic Monte Carlo (KMC) simulations, and specifically to lattice KMC simulations as prevalently used for surface and interface applications. We will provide worked out examples using the kmcs code, where we highlight the central approximations made in implementing a KMC model as well as possible pitfalls.

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