

1. Record Nr.	UNINA9910133760803321
Autore	Jansen A. P. J
Titolo	An introduction to kinetic Monte Carlo simulations of surface reactions // A.P.J. Jansen
Pubbl/distr/stampa	Berlin ; ; Heidelberg, : Springer, c2012
ISBN	3-642-29488-X
Edizione	[1st ed. 2012.]
Descrizione fisica	1 online resource (XVII, 254 p. 79 illus.)
Collana	Lecture notes in physics, , 0075-8450 ; ; v. 856
Disciplina	518.282
Soggetti	Monte Carlo method Numerical analysis
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Introduction -- Stochastic Model for the Description of Surface Reaction Systems -- Kinetic Monte Carlo Algorithms -- How to Get Kinetic Parameters -- Modeling Surface Reactions I -- Modeling Surface Reactions II -- Examples -- New Developments -- Glossary -- Index.
Sommario/riassunto	Kinetic Monte Carlo (kMC) simulations still represent a quite new area of research, with a rapidly growing number of publications. Broadly speaking, kMC can be applied to any system describable as a set of minima of a potential-energy surface, the evolution of which will then be regarded as hops from one minimum to a neighboring one. The hops in kMC are modeled as stochastic processes and the algorithms use random numbers to determine at which times the hops occur and to which neighboring minimum they go. Sometimes this approach is also called dynamic MC or Stochastic Simulation Algorithm, in particular when it is applied to solving macroscopic rate equations. This book has two objectives. First, it is a primer on the kMC method (predominantly using the lattice-gas model) and thus much of the book will also be useful for applications other than to surface reactions. Second, it is intended to teach the reader what can be learned from kMC simulations of surface reaction kinetics. With these goals in mind, the present text is conceived as a self-contained introduction for students and non-specialist researchers alike who are interested in entering the field and learning about the topic from scratch.

