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**Effects of surface topography on the collective diffusion of interacting adsorbed particles.**  
(English) [Zbl 1400.82257](#)  
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Summary: Collective diffusion of particles with repulsive nearest-neighbor interactions on bivariate surfaces is studied through Monte Carlo simulation, in the framework of the Kubo-Green theory. Shallow and deep adsorbing sites form  $l \times l$  patches distributed at random or in chessboard-like ordered domains on a two-dimensional square lattice. The influence of the energetic correlation and the lateral interactions on the jump and collective diffusion coefficients are analyzed by simulating the coverage fluctuations in the grand canonical ensemble and the mean-square displacements of particles in the canonical ensemble. The combination of topography and lateral coupling is shown to produce interesting effects such as different filling regimes as well as strong effects on the coverage dependence of the transport coefficients.

**MSC:**

82C80 Numerical methods of time-dependent statistical mechanics (MSC2010)  
65C05 Monte Carlo methods

**Keywords:**

diffusion; adsorption; heterogeneous surfaces; Monte Carlo simulations

**Full Text:** [DOI](#)

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