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Temperature programmed desorption of a binary gas mixture

NAYELI ZUNIGA-HANSEN, M. MERCEDES CALBI, University of Denver —
Temperature programmed desorption (TPD) is an experimental technique that is widely used to determine the adsorption properties of a surface. Many existing theoretical studies have focused on the desorption of a single gas species, but the desorption of binary mixtures is a subject that has been relatively less explored. We perform computer simulations of the thermal desorption of binary gas mixtures using a kinetic Monte Carlo scheme. We start with a simple structure formed by a single line of adsorption sites and two species of adsorbates which bind to the surface with different energies. By varying the initial surface coverage, the particle-particle interactions and the concentration of the different adsorbates, we study the kinetics of desorption of the mixture and compare our results to available experimental data.

Nayeli Zuniga-Hansen
University of Denver

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