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Effect of surface morphology on kinetic compensation effect

NAYELI ZUNIGA-HANSEN, Louisiana State University, LEONARDO E. SILBERT, Southern Illinois University Carbondale — The existence of the kinetic compensation effect, observed in many fields of science, continues to be debated and believed to be a mathematical artifact. Recently, we performed a computational study of the thermal desorption of interacting adsorbates from an energetically homogeneous surface and we observed that the kinetic compensation effect indeed occurs to varying degrees depending on interaction strength. However, other factors which may lead to a kinetic compensation effect have yet to be explored. In the present work, using kinetic Monte Carlo simulations, we study the effects of substrate topology on thermal desorption. We focus on differences between ordered and disordered surfaces at a fixed site coordination number. The rates of desorption depend on surface configuration due to the inherent differences in the local environments of adsorbing sites. While the compensation effect persists for the disordered substrate, it is more strongly influenced by variations in the preexponential factor rather than the activation energy which dominates in the ordered lattice. We expect our results to provide a deeper insight into the microscopic events that originate compensation effects in our system of study but also in other fields where these effects have been reported.

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