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Effect of surface nanostructure on temperature programmed reaction spectroscopy MICHAEL RIEGER, JUTTA ROGAL, KARSTEN REUTER, Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany) — Using the catalytic CO oxidation at $RuO_2(110)$ as a showcase, we employ first-principles kinetic Monte Carlo simulations to illustrate the intricate effects on temperature programmed reaction (TPR) spectroscopy data brought about by the mere correlations between the locations of the active sites at a nanostructured surface. Even in the absence of lateral interactions, this nanostructure alone can cause inhomogeneities that cannot be grasped by prevalent mean-field data analysis procedures, which thus lead to wrong conclusions on the reactivity of the different surface species. The $RuO_2(110)$ surface studied here exhibits only two prominent active sites, arranged in simple alternating rows. Yet, the mere neglection of this still quite trivial nanostructure leads mean-field TPR data analysis [1] to extract kinetic parameters that are in error by several orders of magnitude and that do not even reflect the relative reactivity of the different surface species correctly [2].

[1] S. Wendt, M. Knapp, and H. Over, JACS 126, 1537 (2004).

[2] M. Rieger, J. Rogal, and K. Reuter, Phys. Rev. Lett (in press).

Michael Rieger
Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany)

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