447f Alkali-Promotion in Heterogeneous Catalysis: Dft Study of the Impact of Alkalis on a Number of Elementary Dissociation Surface Reactions

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The outcome of many catalytic processes can be altered dramatically by an introduction of a small amount of various promoters which speed up certain elementary reaction steps, or various poisons which can either slow down particular reaction steps or neutralize catalyst sites that lead to undesired products. For example, alkali promoters are employed to modify activity and selectivity patterns in a variety of heterogeneous catalytic processes. We have employed Density Functional Theory (DFT) calculations to investigate the impact of alkali adsorbates on various elementary reactions on metal surfaces. We have demonstrated that alkali adsorbates induce a substantial electrostatic potential along the z-direction (normal to surface) and significant dipole-like electric fields in the vicinity of the substrates. We show that the alkali-induced electrostatic fields have a crucial impact on the activity and selectivity of a number of technologically relevant catalytic processes. We will illustrate this in a few examples.