



Defects and reactivity in transition metal oxides

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Abstract: Transition metal oxides are central for a wide range of applications. Intrinsic defects are ubiquitous in these materials and can have a marked effect on their properties. In this talk I will first discuss the effect of such defects on the surface reactivity for the example of TiO_2 anatase (101). In order to control these defect-determined properties, one would like to control defect concentrations and locations. I will discuss two routes to achieve this control: By applying electric fields and epitaxial strain. The results of our density functional theory calculations show that such applied external fields can yield both instantaneous as well as permanent control over the defect population, thus being an effective way to tune the defect-induced properties of transition metal oxides.