

Preface

Defects play a dominant role in the rich chemistry and physics of metal oxide surfaces, and which therefore have a profound influence on the burgeoning range of applications. A well-known example concerns titanium oxide, for which the reactive and electronic properties and chemical reactivity stem from variations of stoichiometry. Defects are thought to play a key role in the activity of metal oxides as heterogeneous catalysts or catalytic supports. Moreover, they have been involved in mechanisms of corrosion, geochemistry, gas sensors, microelectronics and many other technological areas as well as the natural world. The large variety of surface defects can be classified into point defects, which involve vacancies, adatoms, interstitial and substitutional atoms, and topological features that include terraces, steps, kinks and corners. Properties of defects are substrate dependent. For instance, excess electrons associated with O vacancies are localised on MgO surfaces but are somewhat delocalised in the case of TiO_2 .

Defects are probed experimentally using a number of tools, for example a point defect can be evidenced by a chemical environment observed via hyperfine electron paramagnetic interactions or by a frequency shift recorded by infrared spectroscopy upon CO adsorption or by a local perturbation seen by scanning probe microscopy (SPM). These experimental studies are guided and informed by extensive simulation work. In the specific case of wide band gap and highly correlated oxides, the choice of the theoretical approach has proved to be an issue. To better describe localized states using the popular DFT approach, a fair amount of work has been dedicated to the development of hybrid functionals and of the so-called DFT+U method in which the Coulomb interaction is partially screened. Through an interplay of theory and experiment it is hoped that properties of oxide surfaces can be tailored for particular applications by adjusting the defect population.

In this book we have collected chapters covering topics such as structural characterization using scanning probe methods, electronic structure, chemical reactivity and subjects related to applications. The latter include catalysis, photocatalysis and resistive switching. Defects on planar surfaces form the focus of much of the book, although the investigation of powder samples also form an important part. The experimental study of planar surfaces opens the possibility of applying the

large armory of techniques that have been developed over the last half-century to study surfaces in ultra high vacuum. This enables the acquisition of atomic level data under well-controlled conditions, providing a stringent test of theoretical methods. The latter can then be more reliably applied to systems such as nanoparticles, for which accurate methods of characterization of structure and electronic properties have yet to be developed. Finally, we would to express our thanks to Chi Lun Pang for his assistance during the editorial process.

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