Connecting theory with experiment: A survey to understand the behaviour of multifunctional metal oxides

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Our ability to understand the physical and chemical behaviour of both structure and processes at the molecular and atomic levels has progressed rapidly over the last three decades, due to development of experimental techniques such as FESEM, STM, HRTEM, EXAFS, XANES, etc., and theoretical methods and computational techniques based on quantum mechanics and statistical mechanics. Theory and experiment each have different strengths and limitations, but these are complementary to a large extent and there is much to be gained by constructing research programs that combine the two. The combined use of theory and experiment permits on the one hand to analyze the many subtle features of the measured data, on the other hand to evidentiate limits and deficiencies of both approaches. Both experiment and theory are indispensable in modern nanoscience and nanotechnology.

The main challenge, when theory and experiment meet, is to find a common language connecting the results obtained by means of these two approaches. The accessibility of the systems to be investigated may be different at the atomic level. On the one hand, a wide range of structures and arrangements can theoretically be explored. In many cases, some of them are impossible to obtain experimentally, but the theoretical analysis provides a full picture of the effects that are present in real systems. After new experimental techniques developed, new experimental data appear, therefore theoretical models are called to help experimentalists to rationalize their results, but also makes predictions that challenge the capability of available experimental techniques in terms of the spatial, time and energy resolutions, and guide experimentalists to design new experiments.

Successful qualitative theories have two important functions. First, theories provide interpretations of the results of experiments and/or calculations that have already been performed. Second, the predictions made by the theories motivate both experimentalists and computational chemists to attempt to validate the theories by testing the predictions made by them. However, in some cases, it is not qualitative theories but the results of high-level calculations that motivate experimentalists to test how quantitatively accurate the calculations are. In other cases calculations are performed to see how well they reproduce experimental results that have already been obtained. When the results of calculations and experiments are found to be at odds with each other, additional experiments and/or calculations almost inevitably follow.

In the present talk, an overview of the results obtained by using this collaborative strategy will be presented, as an effort to achieve a closer look into the atomic level understanding of structure and processes involving multifunctional metal oxides. In particular, three main topics will presented: (i) Surface structure as the key to manipulating the physicochemical properties as well as growth mechanims of nanomaterials, (ii) Characterization of electronic excited states to understand and rationalize optical properties, and (iii) Calculation of three dimensional electron density distribution in materials, as an observable property, determining in whole or in part their physical/chemical properties.