The effectiveness of defective oxides

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Metal oxides are extremely common in our planet. They form the Earth's crust and, on the surface, they participate in a multitude of processes that affect our every day life. This talk will discuss two particular types of metal oxides, namely substituted perovskites and substituted fluorite type oxides. These substituted oxides are intrinsically defective, with multiple oxidation states of the metals, oxide-ion vacancies, and generally a large concentration of defect sites. I will discuss bulk and surface properties, as well as applications in fuel cell and sensors devices.

As a starting point, DFT calculations showing the structure of Sm doped ceria (SDC), namely what is the arrangement of dopants and vacancies in the bulk and on the surface of these materials will be presented. Synchrotron experiments and calculations of electronic structure and characteristics of O^{2-} transport mechanisms will also be discussed. This provides a baseline for the understanding of defective oxides. Then, the more complex perovskite structure of substituted $SmFeO_3$ will be introduced. This family of perovskites shows a great range of properties with multiple potential applications. $Sm_{1-x}Ce_xFe_{1-y}B_yO_{3-d}$ (B=Ni, Co, Cr) materials have been prepared and characterised. These materials show highly tuneable properties, particularly in regards to conductivity and reactivity. As an example, we can switch the material from p- to n- type conductivity (and back) by small changes in dopant concentration. Surface characteristics are key to the reactivity of the perovskites and surface properties are often different from the bulk material. Two of the applications of these tunable material include their use in sensor devices for the detection of reducing gases (like hydrogen, methane and carbon monoxide) and as carbon resistant anodes for low-temperature solid oxide fuel cells. Promising results of these applications will be shown.