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Review

Recent progress in investigations of surface structure and properties of solid oxide materials with nuclear magnetic resonance spectroscopy

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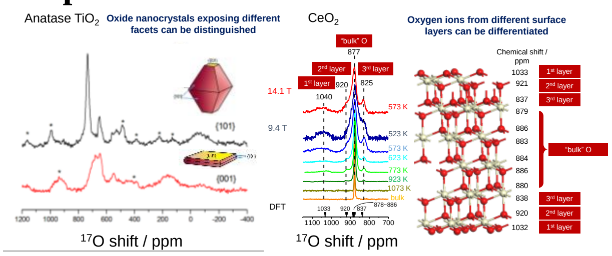
Graphical Abstract



In this mini-review, some of the latest research developments on the characterization of the structure and properties of oxide materials by applying solid-state nuclear magnetic resonance spectroscopy (NMR), including the use of dynamic nuclear polarization (DNP) NMR, ^{17}O NMR combined with surface selective labeling and ^{31}P NMR coupled with phosphorous-containing probe molecules, are discussed.

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ABSTRACT

Solid oxide materials have widespread applications which are often associated with their surface structure and properties. Solid-state nuclear magnetic resonance (NMR) spectroscopy is one of the most powerful methods that give detailed local structural information of solid materials. Recent developments in dynamic nuclear polarization (DNP) NMR spectroscopy and ^{17}O surface-selective isotopic labeling provide more opportunities in investigations of surface structure and properties of oxide materials. We describe in this mini-review some of the latest progress in this field. DNP NMR can enhance the sensitivity of surface sites on the oxides by one to two order of magnitude, making very low concentrated species on the surface of oxides visible in NMR spectroscopy. On the basis of surface-selective ^{17}O isotopic labeling, ^{17}O NMR spectroscopy is now able to distinguish surface oxygen species on the different facets or different surface layers in oxide nanostructures. The nature of these facets can also be probed with help of ^{31}P NMR spectroscopy along with phosphorous-containing probe molecules.

1. Introduction

A variety of technologically important solid oxide materials are extensively used in catalysis [1], energy storage [2], and environmental management [3]. In many cases, their surface structure and physicochemical properties play an important role in controlling the performances in these applications. Recent advances in nanotechnology show that the detailed surface structure of nanomaterials, such as the exposed facets of oxide nanocrystals, have enormous impacts on the catalytic activity [4]. Therefore, such information is required in order to extract the structure – property relationships, rationally design and finally generate new oxide materials with well-defined surface structure and improved properties.

Diffraction methods, which provide long range order information, represent the most extensively used methods in characterizing the crystal structure of solids. However, the surface of solids often has a disordered nature and lacks the structural regularity required by diffraction approaches. On the contrary, solid state nuclear magnetic resonance (NMR) spectroscopy is a versatile tool which gives the