UNDERSTANDING FM-AFM IMAGES ON CERIA WITH AB INITIO SIMULATIONS

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Abstract

Ceria (CeO_2) is a rare-earth oxide with important industrial applications in catalysis and solid-oxide fuel cell technology. Acting as a noble metal supporting substrate, ceria enhances the water-gas shift reaction (WGS, $CO + H_2O \rightarrow H_2 + CO_2$), leading to the massive production of hydrogen [1]. FM-AFM represents the perfect tool for improving our understanding of the microscopic pathways in the WGS reaction [2]: it offers different channels of information and does not require the particular doping and high-temperature conditions that are necessary for the use of the STM in this wide-gap material. A confirmation of the possibilities offered by this methodology comes from recent work where a combination of FM-AFM topography and dissipation images provide the basis to locate sub-surface oxygen vacancies and to show convincingly their local ordering [3].

We have performed an extensive set of ab initio simulations in order to contribute to the understanding of the image contrast, the identification of the observed defects (including oxygen vacancies, adsorbed water molecules and hydroxyl groups) and the interpretation of recent manipulation experiments. Our calculations involve the characterization of the stoichiometric and the reduced surfaces, and the calculation of the tip-sample interaction for different tip models. These calculations are based on approximate DFT+U methods (as implemented in VASP [4]), where the corresponding functional (LDA, GGA) is corrected with the addition of an effective repulsive interaction fitted to reproduce accurate results from hybrid functionals [5,6].

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References:

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