Compensation Mechanisms and Functionality of Transition Metal Oxide Surfaces and Interfaces: A Density Functional Theory Study

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Abstract The valence discontinuity at transition metal oxide surfaces and interfaces can lead to properties and functionality that are not observed in the respective bulk phases. In this contribution we give insight from density functional theory calculations on the emergence of conductivity and magnetism at the interfaces between (nonmagnetic or antiferromagnetic) insulators like $LaTiO_3$ and $SrTiO_3$ as well as $LaAlO_3$ and $SrTiO_3$, and investigate systematically the influence of water adsorption on the surface properties of Fe_3O_4. Additionally we present benchmarks for the performance of the full-potential linearized augmented plane wave method as implemented in the WIEN2k-code on HLRBI and HLRBII.

1 Introduction

The surfaces and interfaces of transition metal oxides represent a natural disruption of the bulk charge neutrality and a multitude of unexpected properties have been observed that differ substantially from the ones of the corresponding bulk materials. In

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