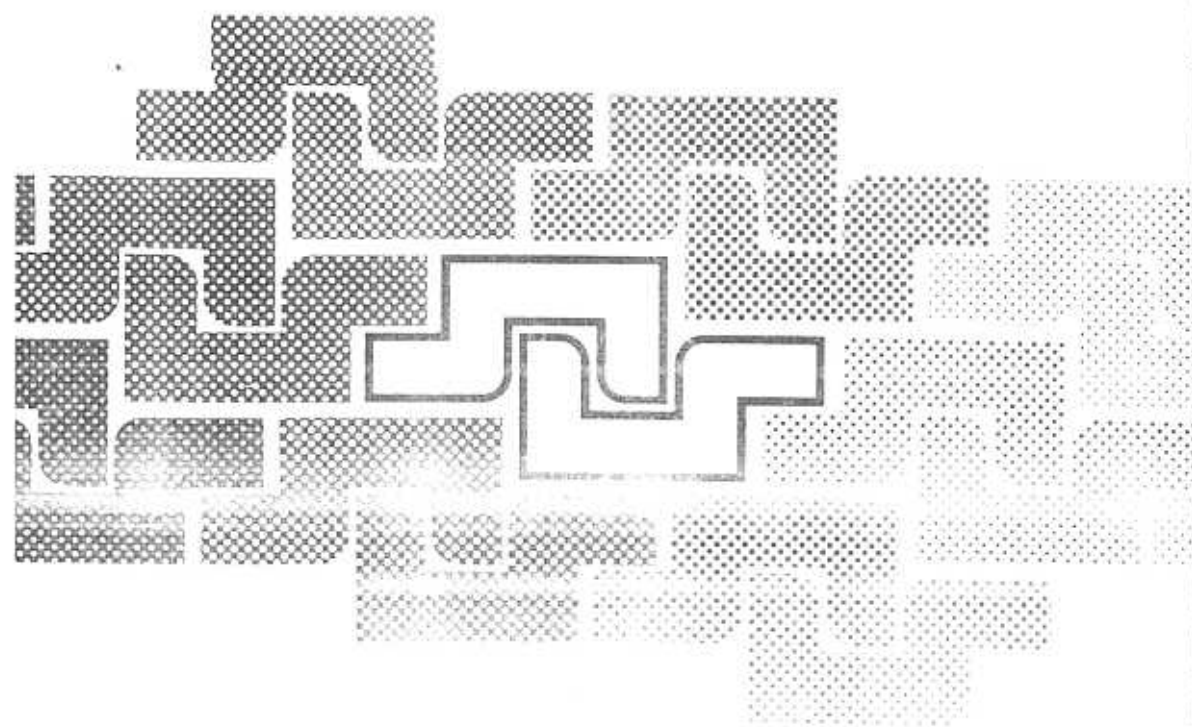




Nanostructured Materials and Coatings for Biomedical and Sensor Applications

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REHYBRIDIZATION AT (110) FACES OF SnO_2 -BASED GAS SENSOR

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1. Introduction

Tin dioxide (SnO_2) is a wide-gap semiconductor with applications as gas sensor material and catalyst. The structure and electronic properties of its surface have been experimentally studied in detail [1, 2]. Also theoretical investigations of oxide surfaces based on an accurate first-principles calculations have been carried out [3–6]. Such approaches allow one to create an atomistic picture of sensing mechanisms and methods for prognosis of gas response properties of the semiconducting materials.

However, *ab initio* calculations of SnO_2 (110) face based on utilizing the different computational methods reveal diversity of bare surface relaxation data [3–6]. Therefore, calculations based on different methods are welcome, to establish reliable structure of relaxed SnO_2 (110) atomic plane and to understand the related differences in rehybridization occurring at stoichiometric and reduced surfaces.

Recently, we have investigated the structure of the (110) face of rutile structure SnO_2 (cassiterite) with *ab initio* – DFT calculations, the local-density approximation (LDA) and the generalized-gradient approximation (GGA) [5]. There are also semi-empirical approaches available for the surface relaxation and electronic structure of the (110) face of SnO_2 to compare with [10].

In the present study, by comparing with the *ab initio* data, we search for the best fitting Universal force field (UFF) of Rappe et al. [8], where the hybridization is explicitly assigned to the atoms. Such comparison of the data from *ab initio* calculations and results of molecular mechanics (MM) minimization allows one to judge between the various presupposed hybridizations.

A more detailed analysis of the hybridizations based on our *ab initio* electronic structure results [5] has been included here, too. The Mulliken population analysis of the