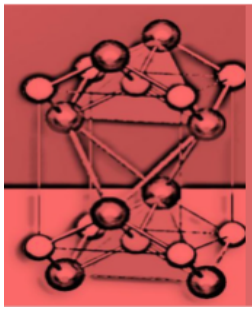

X Workshop on Novel Methods for Electronic Structure Calculations

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Low dimensional structures derived from $A_2Ti_nO_{2n+1}$ (n=1-9, A=alkali metal or H) layered titanates and titanium oxides.

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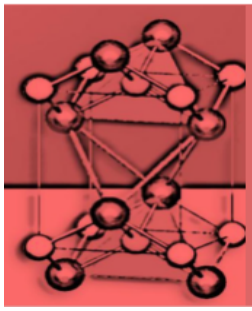
Since first synthesized by Kasuga et al [1], titania and titanate nanostructures have been extensively investigated given their novel properties and potential applications. They have been characterized in terms of ion-exchange properties, proton conductivity, photocatalytic properties, lithium transport and photovoltaic behavior, showing promising results. Particularly given their high surface area and electronic structure, they are interesting for preparing photoelectrodes to dye sensitized solar cell applications (DSSC).

Despite numerous efforts regarding the synthesis and characterization of titanium dioxide and titanates nanotubes and nanostructures, there is still an open debate about their composition and structural characterization, which are crucial to understand their physical properties and surface reactivity. The aim of our line of research is to contribute to the elucidation of crystal structure (building blocks), geometrical parameters and physical properties of high aspect to ratio titanate nanostructures by looking for experimental- theoretical correlation.

We propose modified bulk phases and two-dimensional models derived from titanium dioxide consistent with experimentally observed nanosheets [2], which can also be a first level of approximation of the walls of larger nanotubes. It is in progress the modeling of this type of structures for the case of lamellar titanates of hydrogen, sodium, and lithium; evaluating structure, reactivity, and optical properties, for which an important volume of experimental results has already been obtained by our group [3-7].

Also, from the fundamental point of view, we model one-dimensional structures such as nanowires with a few angstroms in radius, for which there is experimental evidence. In this type of structures, most of the atoms are found on the surfaces and therefore the superficial and quantum confinement effects that generate important changes in the physical and chemical properties are enhanced. It is intended to deepen the study of these systems [8, 9].

In summary, we will show the application of Density Functional Theory for proposing new crystalline phases with different aspect to ratio characteristics. Through the study of its electronic structure, it will be discussed structural properties, vibrational properties (phonons), surface reactivity and optical properties. All of these with the aim to predict and to explain experimental results on layered titanates and titanium oxides.



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