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Study of Electronic, Thermodynamic and Vibrational Properties of SnO_2 Nanoparticles with Different Stoichiometries and Effect of Nonhydrostatic pressure

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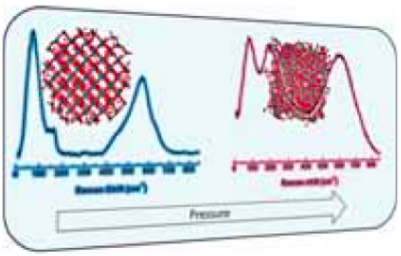
High pressure behavior of SnO_2 nanoparticles of 3 nm is studied up to19 GPa using ab initio method. First, electronic structure equilibrium configuration, elastic and vibrational properties are performed on nanoparticles with different stoichiometries and at normal external pressure. The results are used to evaluate the contribution of the stoichiometry on the surface energy and on the relative stability for different operation condition of temperature and oxygen partial pressure. Secondly, in order to get microscopic description of the shell size and nature of the disorder found with Raman Spectroscopy (RS) in NP of 2.8 nm under high pressure, we introduce in the calculation external non hydrostatic pressure as applied in the RS experiment. The change in the structural properties is analyzed. We calculated for the first time the vibrational density of state of the nanoparticle for different stoichiometries and compared with the Raman spectrum obtained for the same size. The purpose is to know if it is possible to determine the probable stoichiometry of the nanoparticles studied experimentally. In addition, the frequencies of vibration of a free nanoparticle in one spheroidal mode are calculated in the frozen phonon approach.



Recent Publications

1. H.T. Girão, T. Cornier, S. Daniele, R. Debord, M.A. Caravaca, R.A. Casali, P. Mélinon, D. Machon, Pressure-Induced Disordering in SnO2 Nanoparticles, J. Phys. Chem. C 121, 15463 (2017).
2. CA. Ponce, M.A. Caravaca, R.A. Casali, Ab Initio Studies of Structure, Electronic Properties, and Relative Stability of SnO2 Nanoparticles as a Function of Stoichiometry, Temperature, and Oxygen Partial Pressure, J. Phys. Chem. C 119, 15604 (2015)
3. CA. Ponce, M.A. Caravaca, R.A. Casali, Mechanical anisotropy and thermoacoustic properties of SnO2 under high pressures: an ab initio approach, High Press. Res. 34, 205 (2014).
4. R.A. Casali, J. Lasave, M.A. Caravaca, S. Koval, C.A. Ponce, R. L. Migoni, Ab initio and shell model studies of structural, thermoelastic and vibrational properties of SnO2 under pressure, J. Phys. Cond Matter 25, 135404 (2013)

Biography

In memory of Ricardo A. Casali, who was our respected and enthusiastic collaborator. He was completed his PHD at IFLISYB Universidad Nacional de La Plata, Argentina and postdoctoral studies at AARHUS University of Denmark and at IHP at Frankfurt Oder Germany . He was Director of different projects of PHD students and referee of scientist journals. He was Professor at Universidad Nacional del Nordeste, Argentina and published more than 25 papers in reputed journals. He began his theoretical studies describing the static and dynamic properties of semiconductors with point and complex defects, thermoelastic properties of high hardness oxides and was currently applied to describe the electronic thermodynamic, vibrational properties of SnO2 and TiO2 nanoparticles with differents stoichiometry, their relative stabilities and the effects of the pressure on them.

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