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Raman and IR Spectroscopy of SnO_2 Nanostructures with Oxygen Vacancies: An Ab-Initio Calculations

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Abstract

Recent trend and opportunity in the field of transparent and conducting oxides (TCO) based on creation of gaz sensors devises boosted the research to study the large band gap semiconductors like SnO_2, TiO_2 and ZnO. In particularity, tin oxide SnO_2 semiconductor is an important material of transparent and conducting oxides (TCO). has been studied intensively experimentally and theoretically by many researchers, because of its sensitivity and transparency. Tin oxide SnO_2, in his anatase phase, is a large band gap semiconductor (Eg=3.6eV), with space group $P4_2/mnm$[1]. It has been demonstrated that the presence of oxygen vacancy (VO) has an important effect on the electronic, magnetic and spectroscopic properties. In this context, our investigation subscribed. We present an ab-initio study of Raman and IR spectrum of SnO_2 nanostructures with oxygen vacancies.

Method of calculation and models

Using SCF-LCAO-DFT periodic method at the level of B3LYP exchange and correlation pseudopotentials, implemented in the CRYSTAL17 program [2], we performed effective core pseudo-potential calculations. The basis sets used are: DB-41G for O and DB-21G* for Sn. Configurations adopted for different elements are $4d^{10}\ 5s^2\ 5p^2$ for Sn and $2s^2\ 2p^4$ for O. Supercell of 2x2x2 who contain 48 atoms ($Sn_{16}O_{32}$) is used to create 2(VO) Figure1, with cell parameters: a=b=9.57A° and c=6.38A°.

Results and Discussion

many tests are released to obtain the most energetically stabilized structure of SnO_2 with 2(VO). Obtained structure is represented in figure2. For tetragonal structure of perfect SnO_2 crystal, the irreducible representation of normal vibration modes at the center of the Brillouin zone is given by:

$$\Gamma_{RR} = A_{1g} + A_{2g} + B_{1g} + B_{2g} + E_g + A_{2u} + 2B_{1u} + 3E_u$$

Where Raman active modes are represented by: A_{1g}, B_{1g}, B_{2g} (nodegenerated), and E_u (doubly degenerated), and infrared active modes: A_{2u} and Eu(triply degenerated), A_{2g} and B_{1u} modes are silent. Assignment of (VO)s Raman mode is the aim of this theoretical study.

Raman and IR spectrum of stoichiometric and defected SnO_2 structures are represented in Figure2. Vibration Modes of $Sn_{16}O_{32}$ cell structure with 2(VO), are represented in table1.

Table1: vibrational mode of Raman and IR for $Sn_{16}O_{32}$ cell with 2(VO).

Raman vibrationnel mode	**B_{1g}**	**E_g**	**A_{1g}**	**B_{2g}**
Frequencies (cm^{-1})	177	482	707	827
IR vibrationnel mode	**E_u^2 (LO)**	**E_u^3 (LO)**	**A_{2u} (TO)**	**E_u^1 (LO)**
Frequencies (cm^{-1})	294	351	498	706

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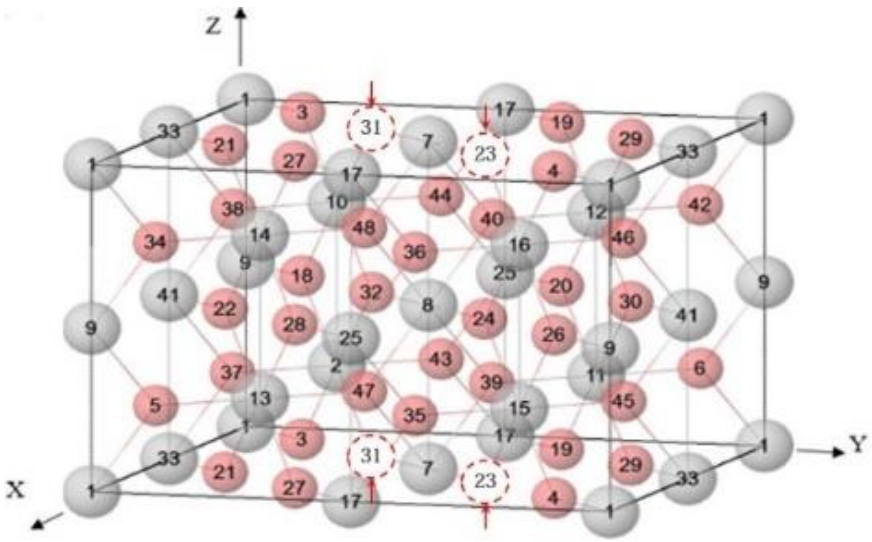
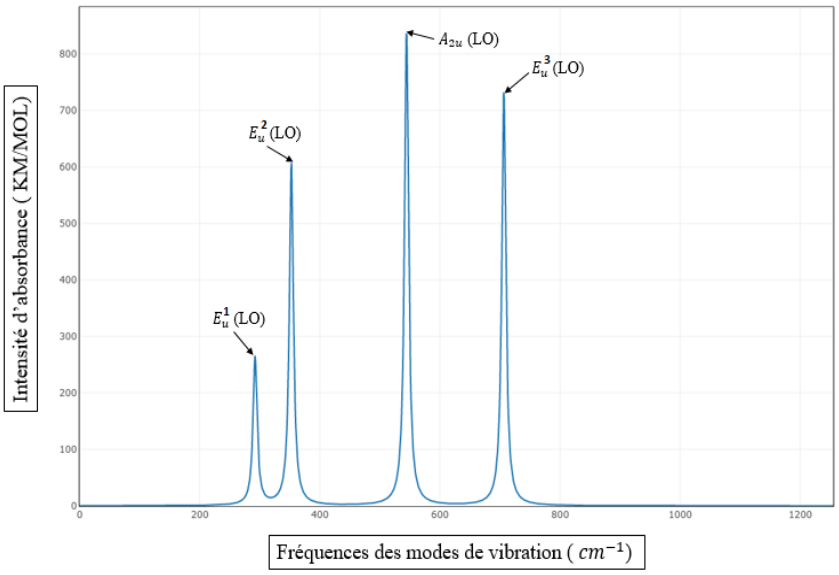


Figure1: $Sn_{16}O_{32}$ cell structure with 2(VO).



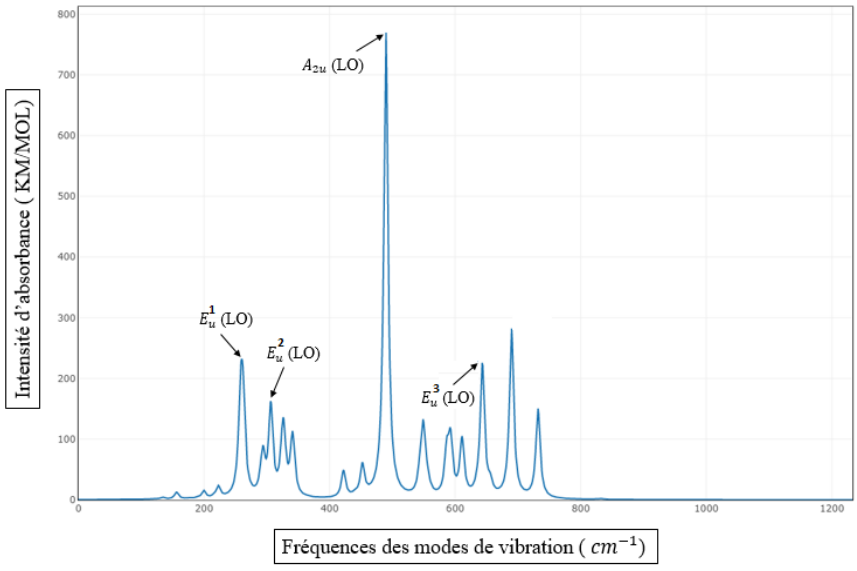


Figure2: IR and Raman spectrum of $Sn_{16}O_{32}$ cell with 2(VO)

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