11th International Conference on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25
ICAM2009

Structural, electronic properties and elastic constants of ZnO

N. L. Marana[(1)*], A. R. de Souza[(1)], J. R. Sambrano[(1)]

[(1)] Grupo de Modelagem e Simulação Molecular, DM e DQ/FC, Unesp, 17033-360 Bauru – SP, Brasil, e-mail: namarana@fc.unesp.br.

Abstract – A theoretical method to simulate the electronic properties, the elastic constants of hexagonal wurtzite ZnO is presented. We report periodic first principle calculations, based on density functional theory with B3LYP hybrid functional and Hartree-Fock using CRYSTAL03 computer code.

Zinc oxide is widely used in technological applications because of its unique electronic and electro-optical properties. Its structural and electronic properties are also of interest because of its importance in catalysis, for example, methanol synthesis. Recently, the successful growth of nanomaterials has increased its potential applications.

The electronic, structural properties and elastic constants of the wurtzite phase of zinc oxide, ZnO, was investigated using computer simulation at Density Functional Theory level, with B3LYP hybrid functional and Hartree-Fock methodology. The electronic properties as well the band energy was investigated through the analysis of the band structures and density of states (DOS), and the mechanical properties was studied through the calculus of the elastic constants C_{11}, C_{33}, C_{44}, C_{12} e C_{13} (Figure 1). The results (Table 1) are in good agreement with experimental data found in the literature and in accordance with results obtained by another theoretical methodology.

Table 1: Elastic Constants (GPa), bulk modulus B (GPa)

	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}	**B****
DFT*	240,09	220,56	65,74	131,83	108,54	**155,40**
HF*	236,10	208,79	62,13	125,32	117,09	**155,55**
HF	246,2	242,5	56,0	127,7	106,2	**157,23**
LDA	217	225	50	117	121	**153,00**
WIEN2k	195,4	199,8	39,6	111,2	116,6	**142,16**
GULP	231	183	72	-	104	**-**
Exp.	**203,2**	**206,9**	**42,86**	**116,6**	**104,8**	**140,63**

*this work, $**B = \frac{2}{9}\left(\frac{C_{11}+C_{12}+2C_{13}+C_{33}}{2}\right)$

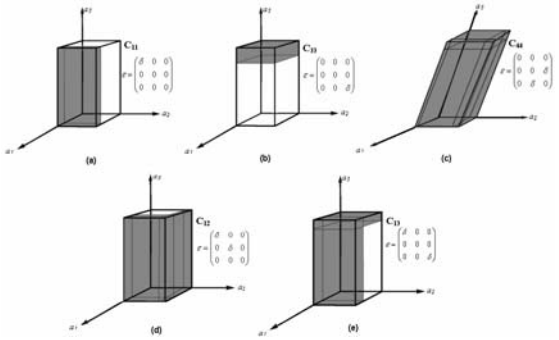

Figure 1: Deformation of the ZnO hexagonal cell, when the strain ε is applied

Acknowledgements: CNPq, FAPESP and UNESP.

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