

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**Structural, electronic, and optical properties of  $\text{Ba}_{1-x}\text{Zn}_x\text{O}$ <sup>1</sup>**

ZEYAD A. ALAHMED, HAMAD A. ALBRITHEN, AHMED M. EL-NAGGAR, Department of Physics and Astronomy, King Saud University, Riyadh 11451, Saudi Arabia — We have investigated structural, electronic and optical properties of  $\text{Ba}_{1-x}\text{Zn}_x\text{O}$  alloy in the range of ( $0 \leq x \leq 1$ ) in the zinc-blende phase. The all-electron full potential linearized augmented plane wave (FP-LAPW) method implemented in WIEN2k code was utilized in these calculations. Structural optimization of  $\text{Ba}_{1-x}\text{Zn}_x\text{O}$  alloy for the compositions  $x = 0, 0.25, 0.50, 0.75,$  and  $1.0$  was carried out by minimizing the total energies as functions of the unit cell volume. The calculated equilibrium lattice constant  $a$  and bulk modulus  $B$  for both binary BaO and ZnO compounds are found to be ( $a = 6.04\text{\AA}$ ,  $B = 45.51\text{GPa}$  for BaO) and ( $a = 4.689\text{\AA}$ ,  $B = 113.84\text{GPa}$  for ZnO), in good agreement with the values reported by different groups. We have observed a nonlinear behavior of the lattice constant  $a$  as varying the composition  $x$ . The electronic structure and the band gap of different composition  $x$  are calculated using different types of exchange–correlation potentials. Additionally, we will present the electron charge density distribution for different crystallographic planes of the unit cell. Also, we will demonstrate the effects of variation of compositions  $x$  on the optical properties such as the complex dielectric function and refractive index of the alloy.

<sup>1</sup>This project is funded by the Saudi National Plan for Science and Technology and King Saud University.

Zeyad A. Alahmed  
Department of Physics and Astronomy,  
King Saud University, Riyadh 11451, Saudi Arabia

Date submitted: 27 Nov 2012

Electronic form version 1.4