

## Electronic States of Impurity-doped ZnO (2)

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We calculated the electronic structures of zinc oxide with various impurity atoms to study energy levels of the impurities in its band gap. Atomic clusters used in the calculations in the present study were based on the following two clusters:  $(XZn_{29}O_{56})$  and  $(XZn_{56}O_{96})$ , whose centers were occupied by O or Zn sites, respectively, where X was an impurity atom from lithium to bismuth without radioactive elements. The calculations of the electronic structure were performed by the discrete-variational (DV)- $X\alpha$  method using the program code SCAT. The energy level diagrams obtained by the calculations of the electronic structures gave us the impurity energy levels. The results showed that all of group VA atoms in the O site such as N, P, As, Sb, and Bi introduced the shallow acceptor levels and that P, S, Ti and so on in the Zn site introduced the shallow donor levels.