

## The p-Type Conduction Mechanism in Zinc-doped Indium Oxide: a Tight-Binding Quantum Chemical Molecular Dynamics Study

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### 【Introduction】

Transparent conductive oxides (TCOs) continue to be in high demand because of their immediate applications. In addition to good quality n-type TCOs, there is increasing demand for good p-type TCOs. In the present study, we reported a theoretical study on the electronic and electrical properties for n-type TCO, Sn-doped In<sub>2</sub>O<sub>3</sub> (ITO), and p-type TCO, Zn-doped In<sub>2</sub>O<sub>3</sub> (IZO). The density of states, molecular orbitals, electrical conductivity, carrier mobility and carrier density of ITO and IZO were calculated by combining the tight-binding quantum chemical molecular dynamics program, “Colors” and Monte Carlo method.

### 【Methods】

To obtain optimum geometries, density functional theory was employed. A novel electrical conductivity estimation method based on our original quantum chemical molecular dynamics program, “Colors” and Monte Carlo method [1] was used to investigate the electrical properties.

### 【Results and Discussion】

In the present study, the electrical and electronic properties of In<sub>32</sub>O<sub>48</sub>, ITO and IZO were investigated using “Colors” program. Fig. 1 shows the calculated total density of states (TDOS) for non-doped In<sub>2</sub>O<sub>3</sub> (a), and Zn-doped In<sub>2</sub>O<sub>3</sub> (b). In comparison with the TDOS of non-doped In<sub>2</sub>O<sub>3</sub>, a dopant level was observed just above the top of the valence band of Zn-doped In<sub>2</sub>O<sub>3</sub>. The appearance of this new feature would explain the reason of p-type conductivity. The electrical conductivities of In<sub>32</sub>O<sub>48</sub>, ITO and IZO were calculated to be  $2.21 \times 10^{23}$ ,  $8.6 \times 10^2$  and  $6.4 \times 10^3 \Omega^{-1} \text{cm}^{-1}$ , respectively. Comparing the electrical conductivity ( $\sigma$ ) of In<sub>2</sub>O<sub>3</sub> with those of IZO and ITO, it is obvious that  $\sigma(\text{In}_2\text{O}_3) \ll \sigma(\text{ITO}) < \sigma(\text{IZO})$ . Our results show that the electrical conductivity increased by introducing acceptor or donor type impurities. Furthermore, the similar large electrical conductivity of p-type IZO and n-type ITO obtained by our new methodology is consistent with study by Phillips et al. [2]. Meanwhile the carrier density and mobility of ITO and IZO were also calculated. The carrier density of IZO is found to be 6.4 times of that of ITO, while the carrier mobility of IZO is close to 0.9 times of that of ITO. Thus, our results indicated that the carrier density dominated the order of conductivity. As a result, we confirmed that our tight-binding quantum chemical calculation method is very effective computational tool for developing and designing both n-type and p-type TCO with high calculation speed.

### References:

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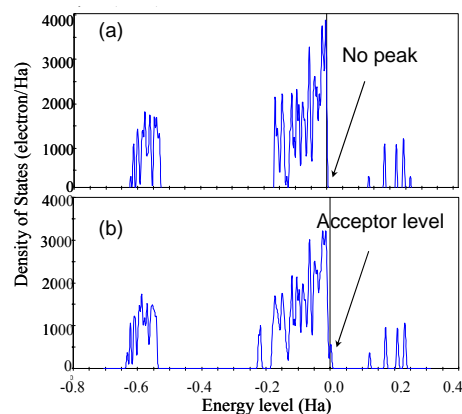


Fig. 1 TDOS for non-doped In<sub>2</sub>O<sub>3</sub> (a), and Zn-doped In<sub>2</sub>O<sub>3</sub> (b).