2O06

Electrical Conductivity of ITO Surface and ITO/Organic Compound Interface: a Tight-Binding Quantum Chemical Molecular Dynamics Study

○Chen Lv[1], Agalya Govindasamy[1], Hideyuki Tsuboi[1], Michihisa Koyama[1], Akira Endou[1], Momoji Kubo[1,2], Carlos A. Del Carpio[1], and Akira Miyamoto[1,3]

[1]Grad. Sch. Eng., Tohoku Univ. (6-6-11-1302 Aoba, Aramaki, Aoba-ku, Sendai 980-8579)
[2]JST-PRESTO (4-1-8 Honcho, Kawaguchi, Saitama 332-0012)
[3]NICHe, Tohoku Univ. (6-6-10 Aoba, Aramaki, Aoba-ku, Sendai 980-8579)

【Introduction】

Because of the increasing interest in the interaction of light with electricity and electronically active materials, transparent electrically conducting films are particular attractive. In particular, considerable attention has been devoted to the study of tin doped indium oxide (ITO) with the intention of their utilization in technology. In this study, a theoretical calculation was performed to study the electrical conductivity of ITO series.

【Computational methods】

To investigate the influence of Sn dopant on the electrical conductivity, we used a novel electrical conductivity estimation method based on "Colors" and Monte Carlo method [1].

【Results and Discussion】

The electrical conductivity of large-scale models: indium oxide and ITO with and without oxygen vacancy was calculated by using "Colors" program. In the case of $In_{128}O_{192}$, the 3.70 eV of E_g is in good agreement with experimental value. Following the Fermi distribution, the HOMO that consists of four degenerate orbitals, and the LUMO shown in Fig. 1, are used to estimate the electrical conductivity of $In_{128}O_{192}$. Based on the obtained band gap and Fermi distribution at 300 K, the number of carrier was evaluated. The total electrical conductivity is the summation of electrical conductivity of each molecular orbital. The electrical conductivity of $In_{128}O_{192}$ is 1.0×10^{-28} ($\Omega^{-1}cm^{-1}$). In the similar way, the electrical conductivity of In_2O_3 with oxygen vacancy, ITO and ITO with oxygen vacancy were obtained. The electrical conductivity for $In_{128}O_{192}$ with oxygen vacancy, ITO and ITO with oxygen vacancy is 1.7×10^{1}, 1.1×10^{2}, and 1.4×10^{2} ($\Omega^{-1}cm^{-1}$) respectively. The electrical conductivity of ITO with oxygen vacancy is close to experimental ranging from 2.5×10^{3} to 4.3×10^{3} $\Omega^{-1}cm^{-1}$. Our results prove that our method is very effective tool to estimate electrical conductivity. Moreover, the electrical conductivity of ITO surface and the complex interface properties of ITO and organic hole-injection film will be presented in the conference.

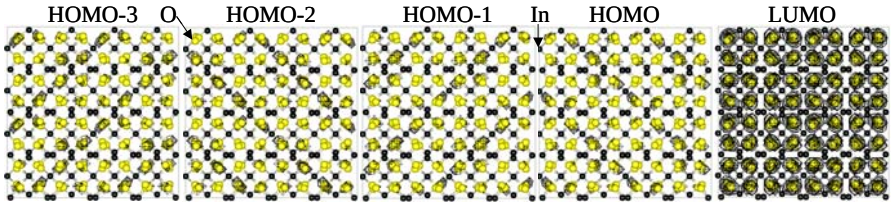

Fig. 1 Density distribution of each molecular orbital of In_2O_3

[1] H. Tsuboi, et al., Jpn. J. Appl. Phys., to be published.