

In₂O₃ 와 Sn-doped In₂O₃ 의 전자 상태 계산 연구
A study on the electronic structure of In₂O₃ and Sn-doped In₂O₃

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Indium oxide film has been widely used for transparent electrodes of solar cells, display devices, etc. A number of research about indium oxide has been made experimentally but few for electronic structure calculation of In₂O₃ has been made theoretically. We investigate the cluster size effect on the electronic state calculation because the band gap is changed with the size of In₂O₃ cluster models. As the size of In₂O₃ cluster increases, calculated band gap is closed to that of In₂O₃ thin films. Thus, it is needed to calculate electronic structure of In₂O₃ clusters and establish an optimum cluster model by comparing the calculated band gap with experimental.

After that, the doping effect of Sn on the electronic structure is calculated using Sn-doped In₂O₃ cluster models. Sn-doped In₂O₃ (ITO) has lower resistivity and higher transmittance (> 85%) in visible light region than the other transparent conductive oxide films such as SnO₂, ZnO, etc. In this research, the electrical and optical properties of Sn-doped In₂O₃ (ITO) is analyzed using the calculated electronic structure of ITO. Sn-doped In₂O₃ (ITO) will be used as a reference material to compare the doping effect of other dopants such as Pb, Zr, Mg, and Zn, etc. on the electronic structure in next research.