

The origin of n-type conductivity in undoped In_2O_3

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This study explored the origin of the native donor in undoped In_2O_3 . The electronic structure of various point defects in In_2O_3 clusters is studied using the first-principles molecular orbital calculation. The results show that an oxygen vacancy cannot act as a native donor, because the defect level formed is much lower than the bottom of the conduction band. However, interstitial indium can generate a shallow donor level, close to the conduction band, and an even shallower donor level is formed when it associates with an oxygen vacancy. It is concluded that the origin of the native donor in undoped In_2O_3 is interstitial indium, but also that the existence of an oxygen vacancy is absolutely essential for carrier generation.