

### A molecular dynamics on the band characteristics of ZnSe thin films

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ZnSe can be applied to the various fields such as laser diode, display, and solar cell, as one of II-VI compound semiconductors which has a wide band gap in the visible region. By using the electrochemical deposition method, ZnSe thin film was synthesized on the ITO glass substrate, where the synthesis of ZnSe and their structure having zinc blende shape were verified through XRD and SEM analysis. By UV spectrophotometric method, the band gap was determined as the value of 2.76eV. Also the band structure of ZnSe grains was analyzed by applying the DFT (Density Functional Theory) in the molecular dynamics. For ZnSe crystals with zinc blende structure, the band structure and its density of state were simulated by using various functionals such as LDA (Local Density Approximation), PBE (Perdew Burke Ernzerhof), and B3LYP (Becke, 3-parameter, Lee-Yang-Parr). Among the calculations of energy band gap upon each functional, the calculated bandgap of 2.65eV value based on the B3LYP functional was mostly near by the experimental one.

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