Theoretical screening of ALD precursors for surface reduction of TiO_2: a density functional theory study

박정우, 엄효빈, 배우진, 송봉근†
홍익대학교
(bshong@hongik.ac.kr†)

2DEG is a group of electrons that exist in a localized thin region at a heterojunction interface, which exhibits high mobility only in the horizontal, in-plane direction. 2DEG is potentially applicable to electronic devices such as HEMTs by taking advantage of excellent carrier concentration and mobility. Recently, a study has been reported that interfacial 2DEG can be formed by ALD of Al_2O_3 on TiO_2 substrate [1]. Experimental evidences suggest that the phenomenon can be due to generation of the partially reduced Ti^{3+} state as the surface oxygen of TiO_2 is removed by the TMA precursor. However, the chemical reaction mechanism between the Al precursor and the TiO_2 surface has not yet been fully elucidated; moreover, other precursor compounds may also have potential to be used to reduce the substrate during ALD. Here, through DFT calculations, we present the chemical mechanism of the formation of oxygen vacancy reaction that appears upon exposure of various Al precursors to the TiO_2 surface. Our study provides a fundamental chemical understanding of the chemical reaction toward generation of 2DEG, and quantitative assessment of viability of the potential Al precursors.