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A hybrid functional study of oxygen interstitial defects in amorphous In-Ga-Zn-O semiconductors[1] WOO HYUN HAN, YOUNG JUN OH, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea — Amorphous indium-gallium-zinc oxide (a-IGZO) semiconductors have attracted much attention because these materials are considered as the replacement of amorphous Si in high performance thin film transistors (TFTs). Although a-IGZO has been the subject of extensive studies due to its superior properties, problems such as threshold voltage shift main as obstacles for device applications. While O-vacancy defects were suggested to be responsible for the device instability under negative bias illumination stress (NBIS), there is no systematic study for the origin of instability under positive bias stress (PBS). In this work, we reveal the origin of PBS instability by performing hybrid density functional calculations for O interstitials in a-IGZO. The defect configuration of an O interstitial depends on its charge state. While an O-O dimer is stable in neutral state, it is easily broken by capturing eletrons, acting as an electron trap. Based on the results for the formation energy and transition level of an interstitial O, we propose that excess O atoms in a-IGZO are responsible for the PBS instability.

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