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**Electronic structure of intrinsic defects in non-stoichiometric amorphous In-Ga-Zn-O semiconductors** WOO HYUN HAN, KEE JOO CHANG, Korea Adv Inst of Sci Tech — Amorphous oxide semiconductors, such as amorphous In-Ga-Zn-O (a-IGZO), have attracted much attention because of their use as a channel material in thin-film transistors (TFTs). Despite many advantages such as flexibility, transparency, and high electron mobility, a-IGZO based TFTs suffer from defects which cause the instability of threshold voltage under negative bias illumination stress (NBIS) as well as positive bias stress (PBS). Recently, we have proposed that O-vacancy and O-interstitial defects are responsible for the NBIS and PBS instabilities, respectively. In the previous studies, O-related defects were intentionally introduced in stoichiometric a-IGZO. Since the composition ratio is likely to be deviated from the ideal stoichiometry during fabrication, it is important to understand the electronic structure of non-stoichiometric a-IGZO. Here we perform density functional calculations to investigate the electronic structure of O-related defects in various a-IGZO systems with non-stoichiometric chemical compositions, which are generated through melt-and-quench molecular dynamics simulations. We consder both O-abundant and O-deficient samples and discuss the role of intrinsic defects in the device instability.

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