First-principles study of structural and electronic properties of amorphous In2O3:Li,Na.

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Amorphous oxide semiconductors (AOS) have found wide application in consumer electronic devices due to their unique properties, namely, high carrier mobility and transparency in the visible. Among the AOS materials, indium-based oxides show best overall performance. Additional cations, such as Zn, Ga, or Sn, allow one to tune the structural, electronic, and optical properties of ternary and quaternary AOS over wide ranges [1-2]. Here we present a thorough systematic analysis of the structural, electronic, and optical properties of amorphous In2O3-x doped with Li and Na. From the theory of glass formation, it is known that alkali metal oxides such as Li2O and Na2O serve as structural modifiers, increasing the materials density. We employ ab-initio molecular dynamics liquid-quench simulations and accurate density-functional calculations to understand how addition of Li or Na affects the local structure as well as the medium-range structure that determines the morphology of the amorphous network. The resulting electronic and optical properties of Li and Na doped amorphous indium oxide are investigated as a function of density, quench rates, cation composition, and oxygen stoichiometry.

[1] J.E. Medvedeva, et al., Adv. Electron. Mater., (2017)

[2] R. Khanal, et al., *PRB*, (2015)