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Long-range structural correlations in amorphous ternary In-based oxides RABI KHANAL, JULIA MEDVEDEVA, Missouri University of Science and Technology — In recent years, there is an increasing shift towards the use of oxide semiconductor materials in their amorphous form owing to several technological advantages and the fact that amorphous oxides exhibit similar or even superior properties than their crystalline counterparts. In this work we have systemically investigated the effect of chemical composition and oxygen stoichiometry on the local and long-range structure of ternary amorphous oxides, namely In-X-O with X=Sn, Zn, Ga, Cd, Ge, Sc, Y, or La, by means of ab-initio molecular dynamics. The results reveal that the local MO structure remains nearly intact upon amorphization and exhibit weak dependence on the composition. In marked contrast, the structural characteristics of the metal-metal shell, namely, the M-M distances and M-O-M angles that determine how MO polyhedra are connected into a network, are affected by the presence of X. Complex interplay between several factors such as the cation ionic size, metal-oxygen bond strength, as well as the natural preference for edge, corner, or face-sharing between the MO polyhedra, leads to a correlated behavior in the long-range structure. These findings highlight the mechanisms of the amorphous structure formation as well as the species of the carrier transport in these oxides.

Rabi Khanal
Missouri University of Science and Technology

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