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Properties of Amorphous Transparent Conducting Oxides from First Principles: In-O, In-Zn-O, In-Sn-O, and Zn-In-Sn-O RABI KHANAL, JULIA MEDVEDEVA, Missouri University of Science and Technology — Systematic investigations of amorphous In-based oxides, In-X-O with X=Zn and/or Sn, obtained via ab-initio molecular dynamics liquid-quench simulations, are performed to understand the role of composition in the structural, optical, transport, and mechanical properties of these oxides. First, the structural characteristics of the first, second, and third shells are compared between amorphous In-O, In-Zn-O, In-Sn-O, and Zn-In-Sn-O. The results reveal that the local Metal-Oxygen structure for both In and X cations – and hence, optical band gap and electron effective mass governed by the metal-oxygen interactions – remains nearly intact upon the transition to amorphous state. In all amorphous oxides considered, Indium is undercoordinated with little dependence on X, whereas the X cations reach their natural coordination. This finding suggests that the carrier generation is primarily governed by In atoms, in agreement with transport measurements in the amorphous oxides. In contrast to the first shell, the composition affects the Metal-Metal distances, coordination, and oxygen sharing. The interconnectivity and spatial distribution of InO6 and XOx polyhedra limits the charge transport via scattering and ultimately determines the formation of the amorphous oxides and their properties.

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