

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First principle study of the role of oxygen non-stoichiometry in the structure and properties of amorphous InO and InGaO.¹ RABI KHANAL, JULIA MEDVEDEVA, Missouri S&T — Ab-initio molecular dynamics liquid-quench simulations of amorphous In-O and In-Ga-O are performed to investigate the structural, electronic and optical properties of these oxides. A new approach is developed to study the formation of oxygen defects in the amorphous oxides and their role in carrier generation and transport. First, the effect of oxygen non-stoichiometry on the local structure (i.e, the average Metal-Oxygen bond length and coordination) as well as on the long-range structural characteristics (i.e., the average M-M distance and the M-O-M angle) is discussed. The latter determines how the MO polyhedra are connected into a continuous network. Presence of Ga has a significant effect on the long-range structural correlations in non-stoichiometric structures. Further, the structural properties of oxygen defects as well as their effect on the electronic band structure is investigated. The results reveal charge accumulation on metal-metal bond(s) near the Fermi level suggesting the existence of two types of oxygen defect. Finally, strongly localized states near the valence band maximum originate from O₂ bonds and from charge imbalance associated with low coordinated oxygen atom surrounded by highly coordinated metal atoms.

¹NSF grant DMR-1121262

Rabi Khanal
Missouri S&T

Date submitted: 06 Nov 2015

Electronic form version 1.4