**Maximizing Electrical Conductivity in Amorphous Oxide Semiconductors**

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Amorphous oxide semiconductors (AOS) with weak metal-oxygen bonding, such as In- or Sn-based oxides, are disordered within the short- and medium-range structure, making every metal-oxygen polyhedron unique in itself and/or its environment. The resulting intricate coordination distribution combined with an increased number of degrees of freedom supports coexistence of extended, weakly localized, and charge trap defects in sub-stoichiometric amorphous oxides and promotes switching between shallow and deeply bound states, invisible to conventional x-ray or electron beam probes and static measurements of carrier concentration and carrier mobility. Lack of microscopic understanding of the origins of oxygen defects with various degree of electron localization, different binding energies, and unique dynamical properties, make the electron transport and optical transmission hard to control experimentally even in commercialized AOS.

In this work, experimentally-validated statistical methodologies that involve ab-initio non-stoichiometric liquid-quench molecular dynamics simulations, advanced time- and temperature-dependent structural analysis, and accurate hybrid-functional calculations are employed to identify, classify, and quantify various oxygen defects in prototype AOS, In2O3-x and SnO2-x. To derive the materials genome of the complex defect formation in these amorphous oxides, multiple descriptors of the defect’s local structure are considered in concert with extended bond reconfiguration that occurs to accommodate the defect in the disordered lattice. The time-resolved behavior sheds light on the defect stability, defect transformations, and defect diffusion. Matching the results with the defect’s ability to induce, compensate, or trap electronic charges, helps detangle the role of specific defects in competing mechanisms for carrier generation, charge scattering, instabilities, and optical absorption. Moreover, we further explore (pre)crystallization-mobility dependence in multi-cation AOS to accurately describe the structure-property relationship in these systems within relevant parameter space.

The results of this work provide practical design principles for next-generation transparent (micro) electronics, *e.g.*, ultra-low leakage switching transistors and high-resolution sensors, MEMS, and for neuromorphic computing applications. The results also help explain unusual quantum behavior, namely, superfluid stiffness in superconducting amorphous indium oxide that raises exciting questions about the role of disorder in quantum phase transitions.