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Transparent Conducting Oxides: Modeling, Understanding, Designing Prof. Julia E. Medvedeva

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Tunable electrical conductivity – the ability to change carrier concentration over a wide range of useful values while maintaining superior mobility – is arguably the central technological advantage of transparent Amorphous Oxide Semiconductors (AOS) such as ternary or quaternary oxides of post-transition metals, for example, In-Sn-O, Zn-Sn-O, or In-Ga-Zn-O. Compared to the crystalline counterparts, wellstudied transparent conducting oxides, where the electron mobility is governed primarily by scattering on ionized impurities, phonons, and grain boundaries, the nature of and the relationship between the carrier generation and transport in AOS are more complex. While amorphous materials lack grain boundaries, the strong local distortions in the Metal-Oxygen (M-O) polyhedra associated with a weak ionic M-O bonding as well as medium- and long-range structural correlations in the disordered system give rise to intricate transport phenomena at different length scales. Moreover, given many degrees of freedom in amorphous oxide, the structural characteristics and the electronic properties of defects in AOS differ fundamentally from those in the crystalline transparent conducting oxides. In this talk, complex deposition-structure-property relationships in several prototype AOS will be discussed. Based on a thorough comparison of the results of ab-initio modeling, comprehensive structural analysis, accurate property calculations, and systematic experimental measurements, we will outline a fourdimensional parameter space for AOSs that serves as a foundation to optimize the properties of known AOSs and to design next-generation transparent amorphous semiconductors.