Fundamentals of Amorphous Oxide Semiconductors

Date : **Friday, October 4, 2019**

Time : **4:00 pm – 5:00pm**

Location : **Neckers 240**

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Abstract:

Amorphous oxide semiconductors (AOSs)—wide-bandgap oxides of post-transition metals such as In-Sn-O (a-ITO) or In-Ga-Zn-O (a-IGZO)—have attracted a lot of attention due to high carrier mobility, which is an order of magnitude larger than that of amorphous silicon (a-Si:H). Unlike Si-based semiconductors, AOSs were shown to exhibit optical, electrical, thermal, and mechanical properties that are comparable to or even superior to those possessed by their crystalline counterparts. Although amorphous materials lack grain boundaries, the electron transport in AOSs is more complex than in the crystalline phases: strong distortions in the metal-oxygen polyhedra and intricate structural morphology in AOSs affect the carrier mobility via composition, defects, thermal vibrations, nano-crystallinity, and lattice strain. Moreover, given the many degrees of freedom in amorphous oxide, defects in AOSs have structural, thermal, and electronic characteristics that differ fundamentally from those in crystalline transparent conducting oxides.

In this talk, complex deposition-structure-property relationships in several prototype AOSs will be discussed. Based on a thorough comparison of the results of ab-initio Molecular Dynamics modeling, comprehensive structural analysis, and accurate density-functional calculations of the properties with systematic experimental measurements, we will outline a four-dimensional parameter space that describes complex microscopic behavior in AOSs, serves as a foundation to optimize the properties of known AOSs, and helps derive versatile design principles for next-generation transparent amorphous semiconductors.

Bio:

Dr. Julia Medvedeva is a Professor of Physics and a Senior Investigator at the Materials Research Center of the Missouri University of Science and Technology. She received her PhD from the Russian Academy of Sciences in 2002, and worked as a pre- and post-doctoral fellow at Northwestern University. She has over 80 publications and a book chapter and is a leader in the area of transparent conducting oxides. Currently, she leads a collaborative materials genome grant funded by NSF-DMREF program and is a co-PI on a NSF-MRI grant to scale-up high-performance computational resources at Missouri S&T.