FEB 12, 2015

Twisted Bilayer and Tri-layer Two Dimensional Metal Chalcogenides: Controlled Synthesis, Characterization, and Optoelectronic Devices

KAI XIAO

Scientist
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN

ABSTRACT:

Characterizing and controlling the interlayer orientations and stacking order of two-dimensional (2D) crystals and van der Waals (vdW) heterostructures is crucial to optimize their electrical and optoelectronic properties. Interlayer interactions play a critical role in the coupled system of twisted 2D vdW heterostructure crystals, which have quite different angle-dependent electronic and optical properties. Here, I will discuss our recent efforts in exploring the synthesis and detailed characterization of 2D metal chalcogenide (GaSe and $MoSe_2$) bilayer and few-layer crystals with various twist angles. First, the scalable synthesis of several of these structures will be discussed through vapor phase deposition techniques. Atomic-resolution Z-contrast scanning transmission electron microscopy (AR-Z-STEM) is used to clearly show atomic-scale images that reveal both commensurate stacking configurations (AA' and AB-stacking) and incommensurate stacking configurations in as-grown 2D bilayer crystals, as well as atomic configurations and terminations of edges and grain boundaries. Nonlinear optical spectroscopy, such as second harmonic generation (SHG), is used to determine the interlayer twist angle and inversion symmetry. Interlayer coupling investigations are probed by photoluminescence (PL) and Raman spectroscopy. Theoretical analysis of the interlayer coupling energetics vs. interlayer rotation angle reveals that the experimentally-observed orientations are energetically preferred among the bilayer crystal polytypes. We find that twisted-layer metal dichalcogenides have altered optoelectronic and electrical properties as compared to their oriented counterparts. Overall, the talk will summarize our recent progress in synthesizing and characterizing twisted few-layer 2D crystals with a wide range of properties and applications as photodetectors and field-effect transistors.

BIOGRAPHY:

Kai Xiao is currently a staff scientist in the Functional Hybrid Nanostructures Group at the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory (ORNL) and a joint faculty of the Department of Electrical Engineering and Computer Science at the University of Tennessee. He obtained his Ph.D. in Chemistry from the Institute of Chemistry, Chinese Academy of Sciences in 2004 on organic and carbon nanotube electronics. At ORNL, his research interests include understanding and controlling the synthesis of thin films and nanostructured materials such as conjugated small molecules/polymers, organic nanowires, carbon nanotubes, and graphene, and investigating their applications in energy-related devices. His research has more recently focused on: (1) synthesis, characterization, and optoelectronic devices of two-dimensional inorganic crystals; (2) solution processing organic and hybrid provskite photovoltaics. He has published more than 70 research papers on international journals.