

Atomic-scale identification of Boson Complexes across Heterogenous Interfaces in 2D Materials

K. Burns,¹⁺ H. C. Barry,¹ C. Smyth,² J. A. Hachtel³

¹*Department of Materials Science and Engineering, University of Virginia, VA, USA*

²*Radiation-solid Interactions, Sandia National Laboratories, NM, USA*

³*Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, USA*

Two-dimensional (2D) compound semiconductors exhibit a range of levels of disorder dependent on their stoichiometry, which can be engineered based on growth conditions, substrate interactions, or atom-by-atom modifications with charged projectiles. There is an entire framework of studies that builds upon research dedicated towards the associated properties with heterogeneities in films, but fail to make one-to-one correlations with the atomic arrangement of the lattice and the optical/infrared emissions. In this talk, we first use aberration-corrected scanning transmission electron microscopy (STEM) to visualize the atomic sites and interfacial growth along semiconducting films. Then, monochromated electron energy loss spectroscopy (EELS) inside an aberration-corrected STEM is used, which greatly reduces the energy distribution of the electron source to maximize the energy resolution without sacrificing too much spatial resolution. Accordingly, we map the high-frequency vibrational modes and exciton complexes in transition metal dichalcogenides (TMDs) moiré structures (Fig. 1) and transition metal monochalcogenides (TMCs) lateral interfaces (Fig. 2). We strategically incorporate off-axis EELS into our workflow, in which it suppressed delocalized responses from Cherenkov radiation losses, to correlate the impact single atom modifications have on the vibrational and optical spectrum. Ultimately, we address applications ranging from magnetic-tunnel transistors to energy harvesting devices.

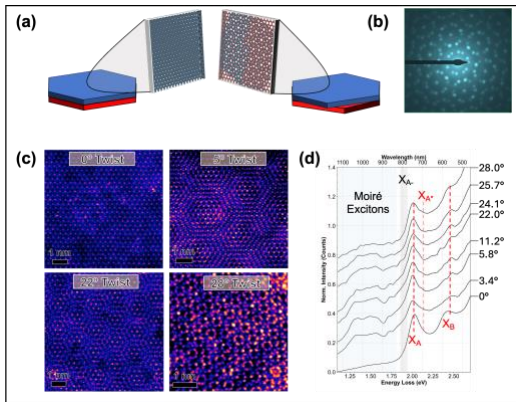


Figure 1: Deformation-field controlled moiré patterns in TMDs. (a) schematic of rotation mismatch. (b) Diffraction pattern of twist angle. (c) STEM images of rotations in TMD bilayers. (d) Moiré excitons in TMDs.

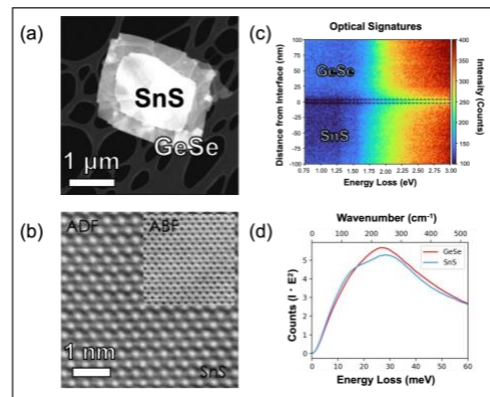


Figure 2: Advanced characterization of SnS-GeSe. (a) STEM image of SnS-GeSe. (b) Atomic resolution image of SnS. (c) EELS map of band edge along interface. (d) Phonons in SnS and GeSe.

⁺ Author for correspondence: koryburns@virginia.edu