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Surface atomic structure characterization of SnSe and black phosphorus using selected area uLEED-IV via LEEM ZHONGWEI DAI, MAXWELL GRADY, JIEXIANG YU, JIADONG ZANG, KARSTEN POHL, University of New Hampshire, WENCAN JIN, YOUNG DUCK KIM, JAMES HONE, JERRY DADAP, RICHARD OSGOOD, Columbia University, JERZY SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory, SURESH VISHWANATH, HUILI XING, Cornell University — Selected area diffraction intensity-voltage (μLEED-IV) analysis via low energy electron microscopy (LEEM) has the combined functionality of atomic surface structure determination and μm area selectivity, making it ideal for structural investigations of 2-D materials. SnSe thin films have been predicted and observed to be topological crystalline insulators. Previous studies suggested that SnSe has a preferred Se-terminated surface configuration. Using μLEED-IV, we determined that SnSe has, on the contrary, a stable Sn termination. This surface is stabilized through an oscillatory interlayer relaxation, which agrees with previous DFT predictions. Black phosphorus (BP) has an intrinsic layer-dependent bandgap ranging from 0.3 eV to 2 eV. Previous STM and DFT studies suggested BP surfaces have a buckling of 0.02 Å to 0.06 Å. We experimentally determined that the surface buckling of BP to be near 0.2 Å. We further propose, using DFT calculations, that this large surface buckling is induced by the presence of surface defects. The influence of this surface buckling on the electronic structures of BP is under investigation.

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