

If any of the two talks gets reassigned to a different section, we request they get reassigned together, in the same order (Zachariah Hennigausen et. al first, Gianina Buda et al. immediately after).

Abstract Submitted
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Ab-initio study of heterostructures of vertically stacked and rotationally aligned incommensurate 2D-films¹ GIANINA BUDA, CHRISTOPHER LANE, ZACHARIAH HENNIGHAUSEN, ANTHONY VARGAS, Northeastern University, FANGZE LIU, Los Alamos National Laboratory, ISMAIL BILGIN, DANIEL RUBIN, SWASTIK KAR, ARUN BANSIL, Northeastern University — Heterostructures obtained through vertical stacking of atomically-thin films are expected to provide a new generation of materials platforms for fundamental science investigations as well as applications. We discuss how one Bi₂Se₃ quintuple-layer (QL) deposited on an MoS₂ trilayer (TL) can stack aligned rotationally with long-range crystallographic order, despite the incommensurability of their lattices to form a new type of well-defined *heterocrystal*. Surprisingly, interaction between the Bi₂Se₃ and MoS₂ layers leads to electronic properties of the heterocrystal that are quite distinct from those of the parent films. We discuss our experimental findings in terms of first-principles computations of electronic and spin-structures, as well as charge densities for heterostructures of Bi₂Se₃ stacked layer-by-layer on MoSe₂ and WS₂ films.

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