

”Ab-initio study of heterostructures of vertically stacked and rotationally aligned incommensurate 2D-films” by Gianina Buda et al.

If any of the two talks get re assigned to a new section, I respectfully request that they get assigned together in the same order (my talk first, followed by their talk).

Abstract Submitted  
for the MAR17 Meeting of  
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**2D Heterocrystals: Vertical stacking of rotationally aligned electronically, structurally and chemically dissimilar 2D materials<sup>1</sup>**  
ZACHARIAH HENNIGHAUSEN, ANTHONY VARGAS, Northeastern University, FANGZE LIU, Los Alamos National Labs, ISMAIL BILGIN, CHRIS LANE, GIANINA BUDA, DANIEL RUBIN, MATTHEW DECAPUA, WENTAO LIANG, ARUN BANSIL, SWASTIK KAR, Northeastern University — We present a new species of 2D materials called ‘Heterocrystals’ (HCs), which are layered stacks of chemically, structurally, and electronically dissimilar 2D materials that grow with perfect rotational alignment and long-range order, despite substantial lattice mismatch. We have successfully grown a family of 2D HCs using chemical vapor deposition. Our investigations reveal a novel lattice matching such that  $n$  unit lengths of one lattice approximately matches  $m$  lengths of the other lattice, e.g.  $3 \times 3$  unit cells of  $\text{Bi}_2\text{Se}_3$  match nearly perfectly with  $4 \times 4$  unit cells of  $\text{MoS}_2$ , forming the larger HC unit cell. The HC exhibits a variety of electronic and optical properties different from its parent 2D crystals. Such large changes in properties are in sharp contrast with those seen from randomly stacked 2D materials, or those grown with high crystallographically commensurate structures. We will present a range of novel, tunable and reconfigurable optical and electronic properties of these new systems, including transition from direct to indirect band gap, tunable and reversible photoluminescences, electronic transport, and Raman spectroscopic results. Our experimental results are in good agreement with theoretical results.

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