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## ABSTRACT:

### Metal to Semiconducting Phosphorous Allotropes on Copper Surfaces Due to Faceting

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Bottom-up growth of 2D materials on high-index surfaces can induce faceting of metallic substrates, leading to the formation of stable facet orientations for specific 2D material–substrate combinations. Different 2D materials may stabilize distinct facet structures on the same substrate. Using the examples of graphene, hexagonal boron nitride, phosphorene, and silicene grown on Pt-like and noble-metal vicinal surfaces, we demonstrate how such stable facets can be investigated through a combination of Low-Energy Electron Diffraction (LEED) and Scanning Tunnelling Microscopy (STM) [1].

In particular, the growth of phosphorus on curved copper substrates shows that only three overlayer–substrate combinations are energetically stable: the (111), (110), and (513) facets. On Cu(111), a metallic blue phosphorene phase has previously been reported [2], whereas on the (513) surface we observe semiconducting phosphorus behavior. This phase has been further investigated using angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations, based on the structural determination of phosphorus obtained from photoelectron diffraction and STM measurements.

[1] AMI Bakhit et al., *Nanoscale* 15, 11517 (2023).

[2] Y. Kaddar et al., *Adv. Funct. Mater.* 33, 2213664 (2023).