Crucial Impact of Substrate Effects on Epitaxially Prepared 2D Transition Metal Dichalcogenides

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At the SGM3 beamline of the ASTRID2 synchrotron light source here in Aarhus, we use an epitaxial approach to fabricate novel single-layer transition metal dichalcogenide systems *in vacuo.* This technique allows us to controllably produce well-oriented single-crystal domains with low defect density. Taking advantage of the high quality of these samples, we have been able to investigate, for a variety of systems based on semiconducting and metallic transition metal dichalcogenides, the complex interactions that emerge between an epitaxial single layer and a metallic substrate. Most importantly, we find that, contrary to simple models in which these single-layer materials interact minimally with their environments, the substrate can in fact play a key role in determining their electronic properties (both band structures and collective ground states) and in controlling what crystalline structures they assume. Indeed, it is even possible to use substrate interactions to realize entirely novel single-layer structures that have no analogue in the bulk. I will present studies based on angle-resolved photoemission spectroscopy, x-ray photoelectron spectroscopy, scanning tunneling microscopy/spectroscopy, and low-energy electron diffraction, and I will discuss how our findings are elucidated by calculations based on density functional theory.