## Phase transition and electronic structure of the antimonene/Bi2Se3 van der Waals heterostructure

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Abstract

The van der Waals heterostructure [1] formed between the 2D trivial semiconductor antimonene (Sb-ene) and the 3D topological insulator bismuth selenide (Bi2Se3) offers a fascinating route for exploring unconventional interfacial phenomena.

In this talk I report on a joint theoretical-experimental study of the growth [2] and electronic properties of single and multilayered Sb-ene on Bi2Se3. STM and ARPES measurements provide evidence for a temperature driven 2D phase transition on the surface, resulting in ordered domains displaying a perfect lattice match with bismuth selenide that can be attributed to stacks of single or double bilayers of buckled antimonene sheets [3]. DFT calculations of the stability and phase transition pathway provide insight into all stages of growth. A delicate interplay between cohesive and van der Waals forces, spin-orbit coupling, strain, and kinetic limiting, emerges. Analysis of the electronic structure yields a clear interpretation of measured spectra in terms of topological surface states induced by proximity effects.

**References:**

[1] K. S. Novoselov et al., “2D materials and van der Waals heterostructures” *Science* , vol. 353, aac9439 (2016).   
[2] R. Flammini et al, “Evidence of β-antimonene at the Sb/Bi2Se3 interface”, *Nanotechnology,* vol. 29, pp 065704 (2018)

[3] C. Hogan et al, “Temperature Driven Phase Transition at the Antimonene/Bi2Se3 van der Waals Heterostructure”, *ACS Nano,* in press, (2019) DOI: 10.1021/acsnano.9b04377