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2023, March 8, 11 a.m.
Room 7

THEORETICAL MODELLING OF THIN ANTIMONY LAYERS ON BI2SE3

Abstract

The antimony on Bi2Se3 system is a van-der-Waals heterostructure consisting of a topologically non-trivial substrate and a topologically trivial adsorbate. While it is clear from the non-trivial Z2 invariant of Bi2Se3 that the heterostructure bears metallic surface states, the detailed origin of the complicated electronic band structure is still unclear. Part of my dissertation [1] addresses this point by density functional theory (DFT) including van-der-Waals corrections and spin-orbit coupling, which both are essential to simulate constituents with such high atomic numbers. At first, stable atomistic models for different Sb coverages are determined by ab-initio thermodynamics. After that, electronic spectra are simulated, evaluated and compared to scanning tunnelling microscopy (STM) and angle-resolved photoelectron spectroscopy (ARPES) measurements. In a last step, a desorption-and-readsorption process is simulated in order to analyse how the Dirac cone of the Bi2Se3 surface combines with the bands of a free-standing Sb sheet to produce the band structure of the heterostructure. This novel approach proves that the first Sb adlayer undergoes a complex series of topological phase transitions upon approaching the Bi2Se3 surface, while a second Sb layer entails a continuous transformation of the bands.

[1] K. Holtgrewe: “Theoretical modelling of nano-scaled systems with heavy ions”, PhD thesis (2022), doi:10.22029/JLUPUB-7899

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European Research Council
Established by the European Commission

Funded by the European Union (ERC, DELIGHT, 101052708)