Manipulation of surface states in topological Weyl semimetal NbP: ARPES study

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Motivation:

Non-centrosymmetric topological Weyl semimetal NbP has two important features, Weyl points (WP) protected at bulk by time reversal symmetry (TRS) and their surface projections, surface Fermi arcs. The interplay between these Fermi arcs and Weyl fermions give rise to many exotic phenonmena such as extremly large magnetoresistance, ultrahigh mobility, quantum oscillations, chiral magnetic effects, etc. Hence it is important to manipulate and control the Fermi arcs [1].

Here, we used surface decoration with heavy metals such as Pb to manipulate the Fermi arcs in the single crystal of NbP and observed the phenomenon by angle resolved photoemission spectroscopy (ARPES).

Single crystal growth and structural analysis:

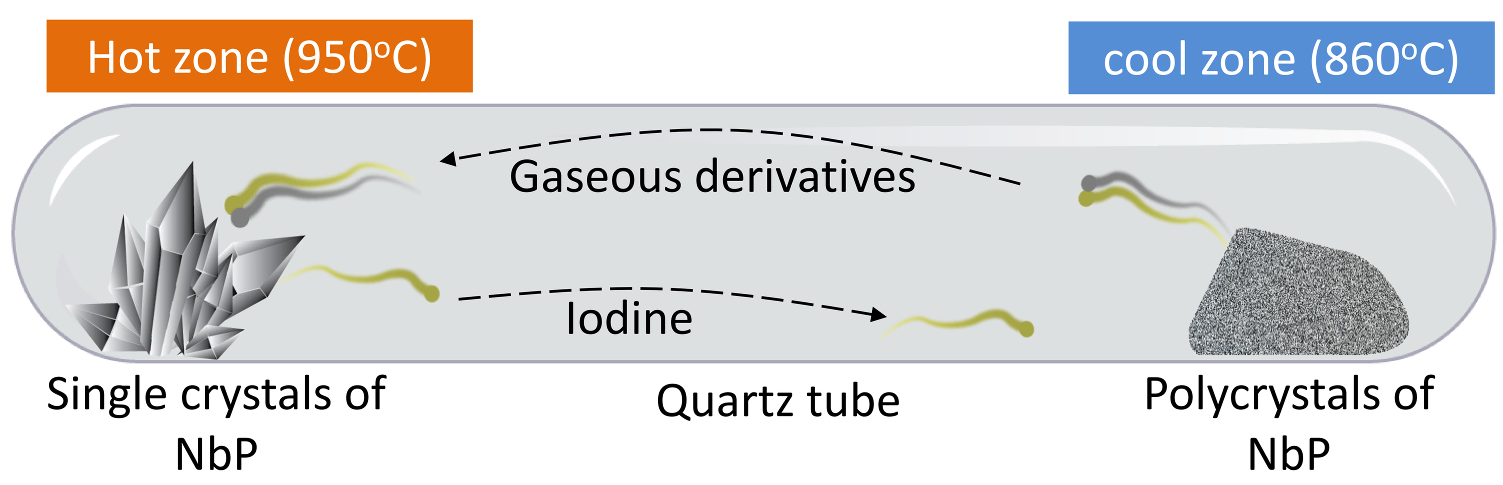


Figure 1. Chemical vapor transport method to prepare single crystals of NbP

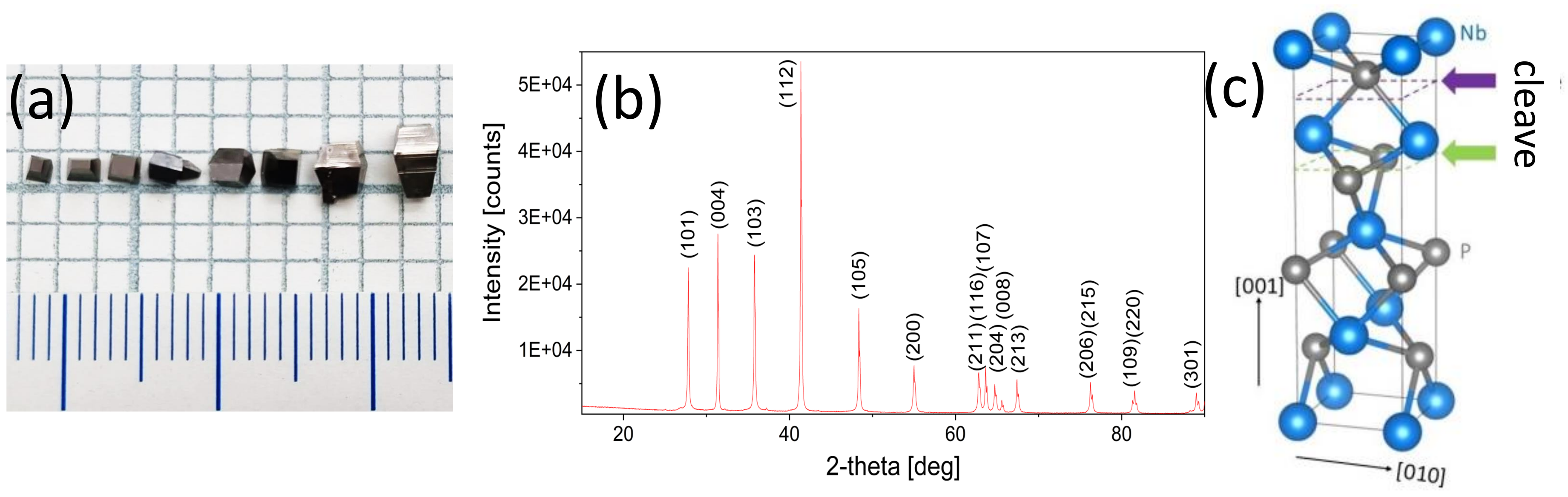
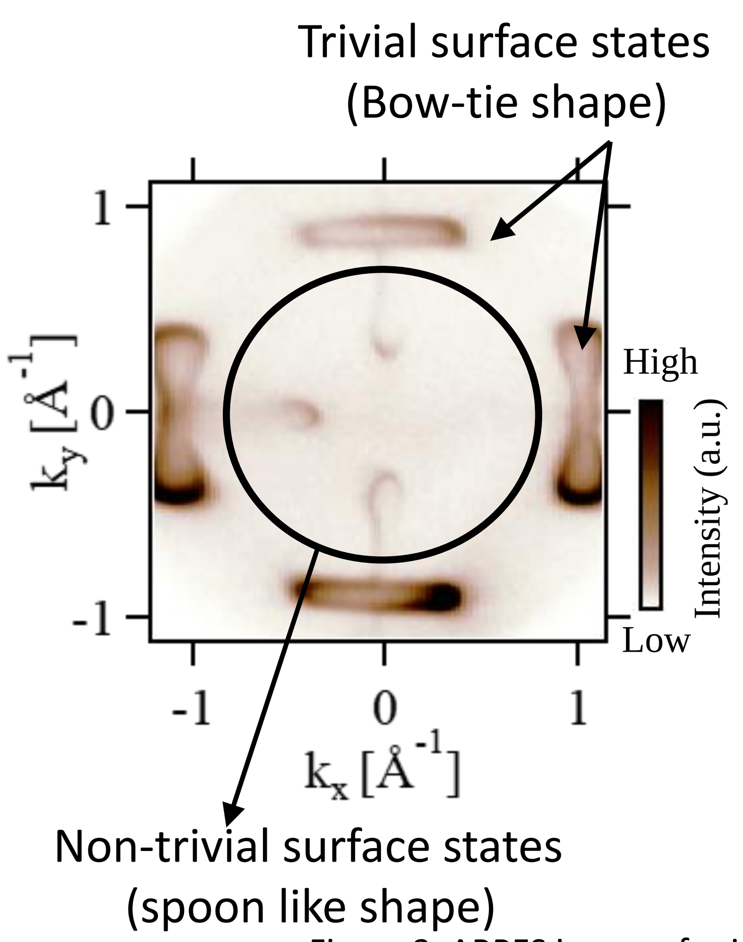


Figure 2. (a) Single crystals of NbP, (b) X-ray diffraction analysis of NbP, and (c) tetragonal crystal structure of non-centrosymmetric NbP

Surface features of NbP:



- NbP have 12 pairs of Weyl nodes in Brillouin zone
- ARPES spectra show a constat energy contour
- Two important surface features:

I. **Trivial surface states:** appear mainly due to presence of dangling bonds on the surface after cleaving the single crystal [2]

II. **Non-trivial surface states:** surface projection of bulk protected Weyl nodes, also called as surface Fermi arcs (SFA) [3]

Photon energy: 90 eV
Temperature : 80 K
Plane Grating Monochromator

Figure 3. ARPES image of pristine NbP showing trivial and non-trivial surface states

Topological Lifshitz transition:

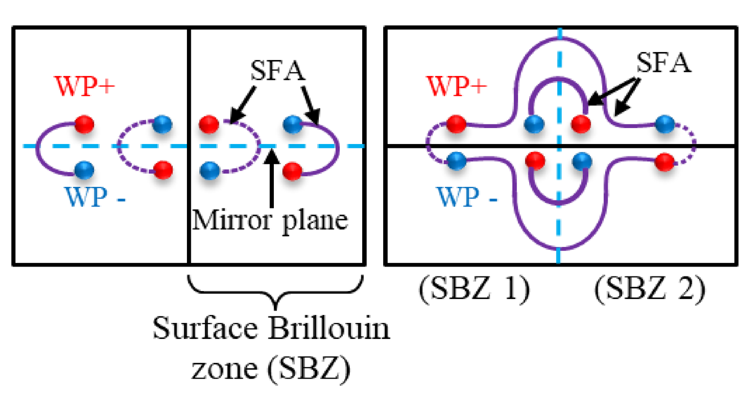


Figure 4. shows topological Lifshitz transition which manipulation of Fermi arcs

- Topological Lifshitz transition (TLT) is a change in the topology of the Fermi surface without breaking of any symmetry [4]
- It is a consequence of external disturbances applied to topological materials due to which the Fermi surface feels the transition
- SFAs change their position from one pair of WPs to another connecting two adjacent surface Brillouin zones

1 ML Pb deposition on NbP:

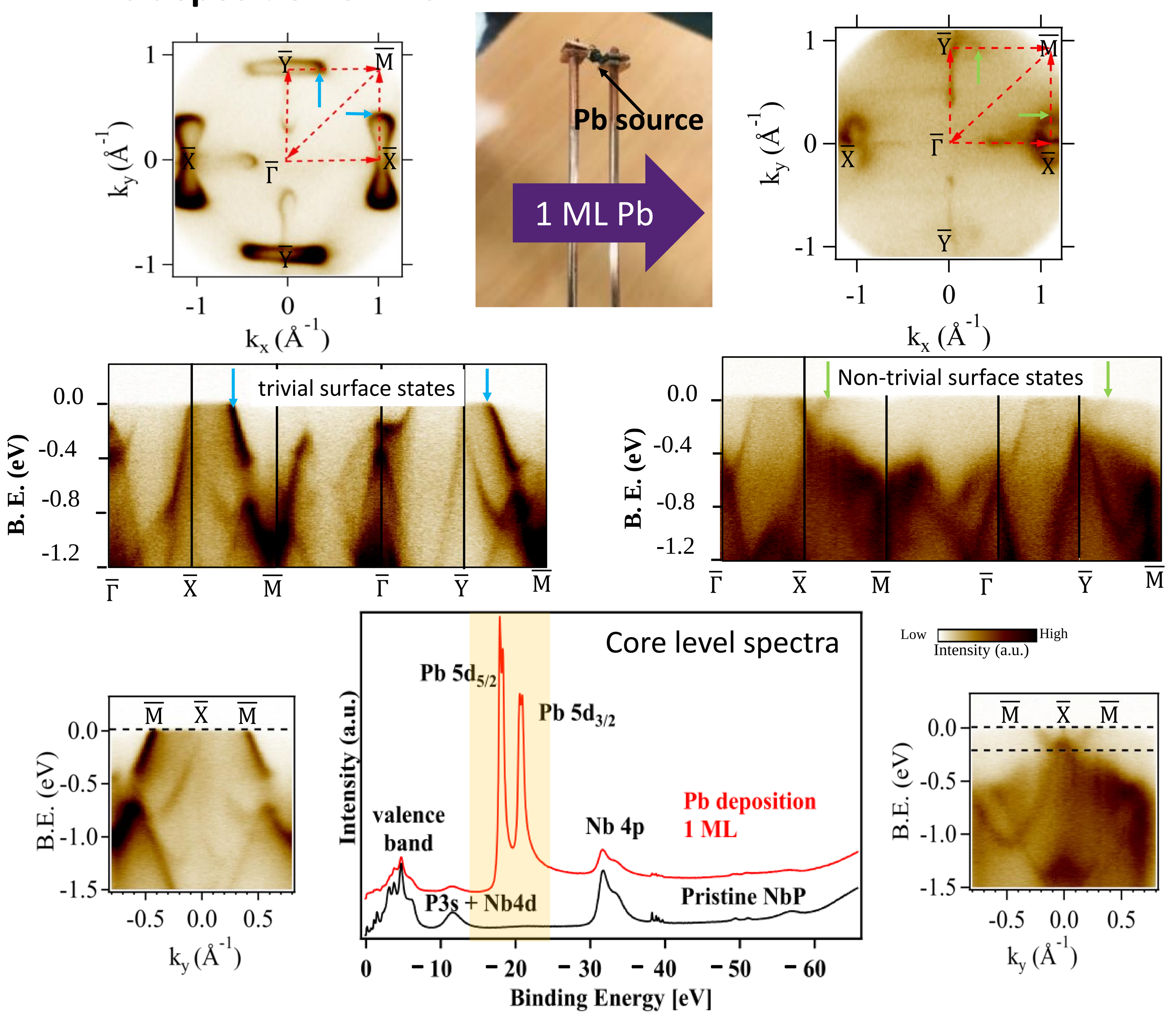


Figure 5. Comparison between pristine NbP and Pb deposited NbP with surface modifications shown at const. E contour and experimental band-structure by ARPES

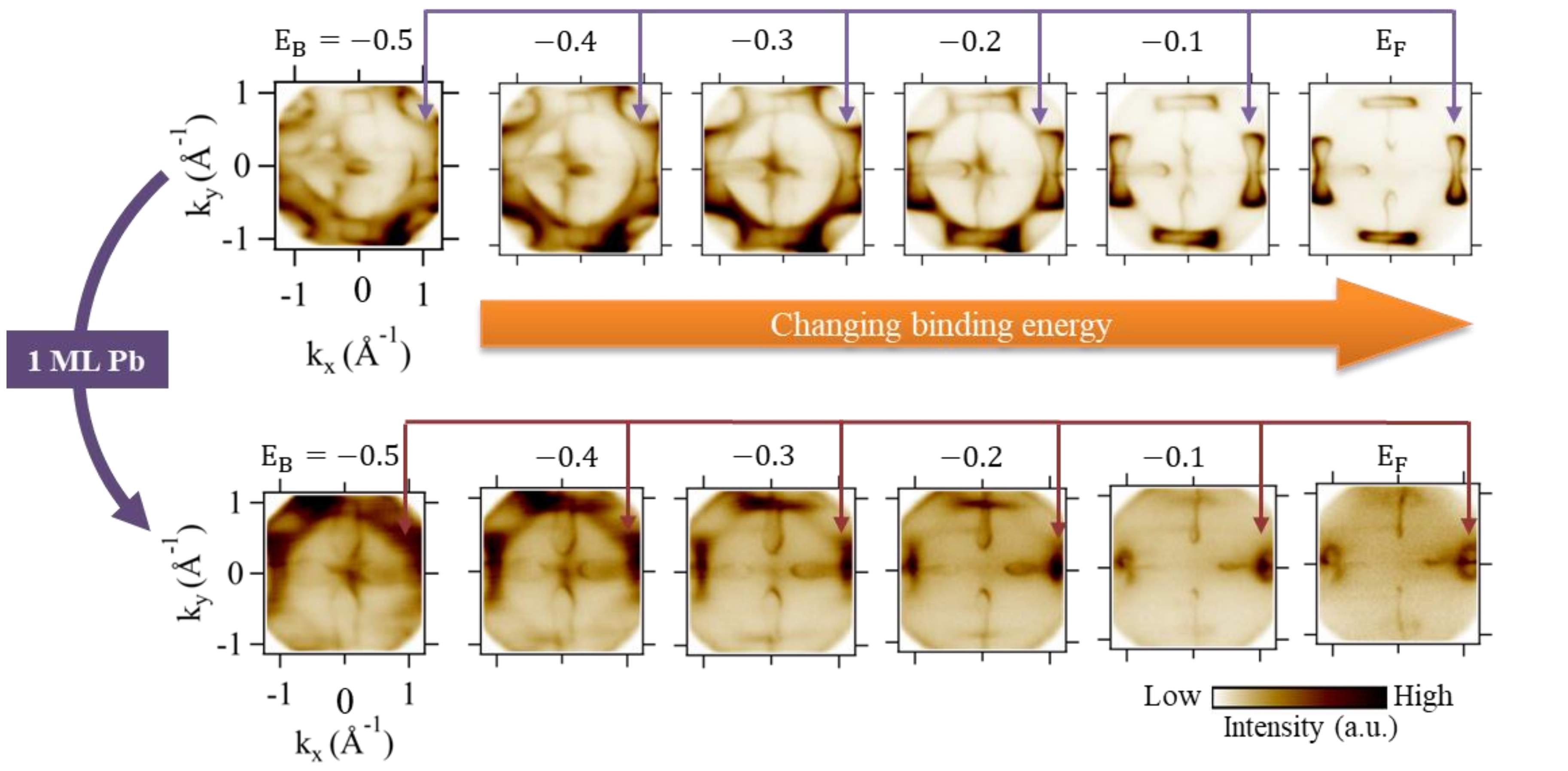


Figure 6. Comparison of 2D Fermi surfaces of pristine P-terminated NbP and 1 ML of Pb decorated P-terminated NbP showing apparent modifications after Pb deposition .

Summary:

- Single crystals of NbP are cleaved in ultra high vacuum (UHV) (in-situ)
- P terminated NbP shows bow-tie like (trivial) and spoon like(non-trivial) surface states in the ARPES spectra
- 1 ML of heavy metal (Pb) deposition on (0 0 1) surface of NbP manipulates the Fermi arcs and changes the band-structure
- Topological Lifshitz transition is responsible for manipulation of surface states.
- Weyl points remain robust against change of surface environment, SFAs remain connected to topologically protected WPs (different pairs before and after TLT)

References:

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arXiv link

Our article on "Topological Lifshitz transition in Weyl semimetal NbP decorated with heavy elements" is accepted in Phys. Rev. B