

Extended Abstract of PSA-19 (review)

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# Electronic Structures of Two-Dimensional Materials

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Energy-tunable synchrotron radiation is essential for angle-resolved photoemission spectroscopy, which is a tool imaging the electronic structure in momentum space. Recently, the 10D HRPES-I beamline of the Pohang Accelerator Laboratory has been considerably upgraded, including the optimization of energy and momentum resolutions, two-dimensional mapping, etc. Here, we provide peculiar electronic structures of 2D layered materials taken at the beamline.

## 1. Angle-Resolved Photoemission Spectroscopy

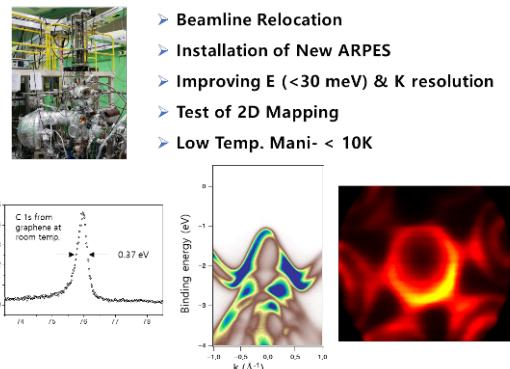
Materials have plenty of atoms and electrons. Atoms and core electrons are localized, whereas valence electrons are delocalized in real space. Important physical properties, for example, transport, optical, magnetic ones, are strongly related with the delocalized valence electrons. How can we get information about them ? Fortunately, they are localized in momentum space. So if we know the structure of valence electrons in momentum space, we could understand where key properties come from. Angle-resolved photoemission spectroscopy (ARPES) is almost the only tool imaging the electronic structure in momentum space [1], whereas microscope, such as transmission electron microscope, scanning tunneling microscopy, etc. can image atoms in real space. Synchrotron radiation is essential for ARPES nowadays, because it is excellent in terms of brilliance, energy-tunability, high resolution, complimentary core level spectroscopy, polarization.

## **2. Upgrade of 10D beamline at Pohang Accelerator Laboratory**

In order to improve the performance, the 10D HRPES-I beamline [2] of the Pohang Accelerator Laboratory (PAL) has been upgraded under the slogan ‘Undulator-like Bending !’ At first, we installed a new ARPES system equipped with the DA30 electron

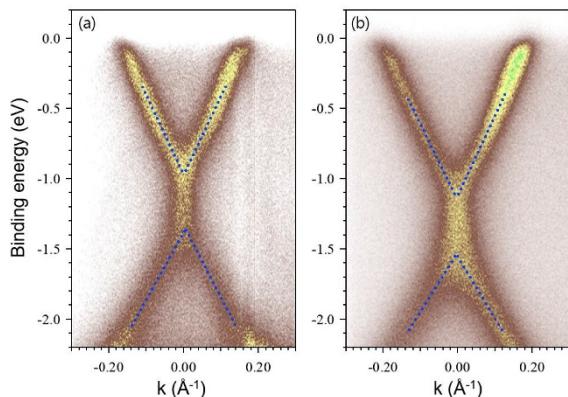
analyser that gives us two-dimensional (2D) mapping capability, as shown in Fig. 1. Second, the beamline was realigned to optimize the energy resolution and the photon flux. We have tried to find a simple and quick way to align it within short time when the electron beam is not in stable status. Third, the new end station was not only positioned at the focal point but also is movable along the direction parallel to the beamline to keep the momentum resolution optimized. Fourth, we have been developing a new sample manipulator working at considerably low temperature. We do not have to rotate the sample to take 2D mapping data, which offers a possibility to lower the sample temperature further. We expect the development to be done soon.

## Advanced ARPES



**Fig. 1** New ARPES set-up recently installed in the beamline.

### 3. Electronic Structure of 2D Materials



**Fig. 2** Electronic structures of the Na (a) and K (b) adsorbed-graphene/Au/Ni(111) surfaces enlarged near the Fermi level and the K point. (Ref. 5).

2D materials show intriguing band structures. In graphene, as an example, its conduction and valence bands meet together at a Dirac point and the energy depends linearly on the wave vector near the K-points. However, it has intrinsically no sizable energy gap and no spin-polarized bands, etc. To overcome the weak points for some applications, we could use MoS<sub>2</sub> with a band gap or WSe<sub>2</sub> with spin-split bands at the K point although they have almost the same atomic structure as graphene [3, 4]. Alternatively, we are able to tune graphene's electronic structure by forming heterostructures for specific applications because real graphenes often show different electronic structures from the simple one depending on what they are facing with. Here, we present intriguing electronic structures of 2D layered materials taken at the 10D beamline of PAL. We compare the ARPES data from graphene, MoS<sub>2</sub>, WSe<sub>2</sub>, etc. In particular, we will show how graphene's electronic structure can change depending on formed heterostructures using scanning tunneling microscopy, photoluminescence, and density functional theory calculation as well as ARPES. For example, Fig. 2 shows the electronic structures of the Na (a) and K (b) adsorbed-graphene/Au/Ni(111) surfaces near the Fermi level and the K point. The bands are not linear anymore and there exists an energy gap of  $\sim 0.4$  eV. This indicates that the graphene is not ideal and considerably interacting with the underlying Au layer with large spin-orbit coupling. Such layered heterostructures could be useful to give a valuable function to 2D materials, such as large spin-orbit coupling [5], magnetism, superconductivity [6], photoluminescence

[7], band gap [8], etc., that are not expected in isolated one.

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