Electronic Structures and Magnetic Properties of the Two-Dimensional Electride Y_2C

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Electrides are ionic crystals in which electrons serve as anions. Recent studies have reported the synthesis of possible two-dimensional (2D) electrides such as Ca_2N and Y_2C. *Ab initio* calculations have predicted that the confined electrons in the interlayer freely move inside this 2D space and consequently form the "2D electride band" near the Fermi level (E_F). The crucial issue in the research of the 2D electrides is whether or not the material concept is really realized in these materials. In order to credibly prove that these candidate materials are indeed a 2D electride, it is necessary to directly probe the electronic band structure. Therefore, we have performed angle-resolved photoemission spectroscopy (ARPES) on a possible 2D- electride material Y_2C.

Figure 1 shows the experimental band structures of Y_2C obtained by ARPES. The measurements are performed at BL-2 MUSASHI synchrotron beamline of Photon Factory, KEK. Clear band dispersions are observed near E_F, which corresponds to the "2D electride bands" in the band structure calculation. The good agreement between the experimental and theoretical results suggests that Y_2C is surely a 2D electride material.

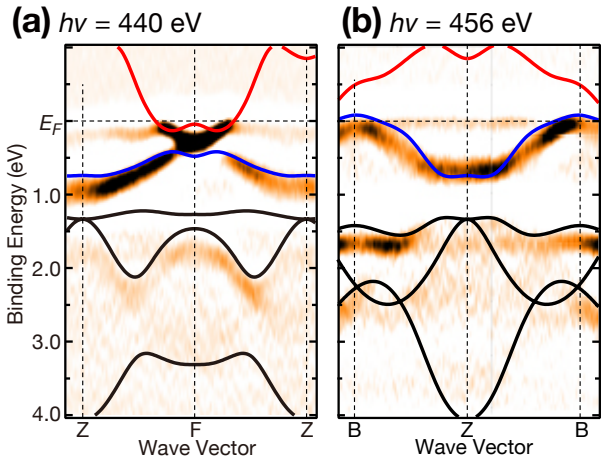

Fig. 1. Experimental band structures of Y_2C measured (a) at $h\nu$ = 440 eV and (b) at $h\nu$ = 456 eV. The energy bands along the Z-F-Z and B-Z-B directions by the theoretical calculations are superimposed by solid lines, respectively.

The magnetic property of Y_2C is still in under discussion. Theoretical calculation [2] suggested an enhancement of the Stoner-type ferromagnetic instability. However, the muon spin rotation (μSR) measurements performed at J-PARC MLF and TRIUMF (Canada) has ruled out any type of magnetic order down to milli Kelvin regime. Instead, existence of paramagnetic local moment was observed in muon Knight shift measurement [3]. The discrepancy between the theory and the measurement may stem from the electronic correlations which may not be included thoroughly in the theory.

Bibliography

[1] K. Horiba, R. Yukawa, T. Mitsuhashi, M. Kitamura, T. Inoshita, N. Hamada, S. Otani, N. Ohashi, S. Maki, J. Yamaura, H. Hosono, Y. Murakami, and H. Kumigashira; Phys. Rev. B, **96**, 045101 (2017).
[2] T. Inoshita, N. Hamada, and H. Hosono; Phys. Rev. B 92, 201109(R) (2015).
[3] M. Hiraishi *et al.*; in preparation.