RIIS Seminar / Physics Department Seminar

異分野基礎研セミナー / 物理教室談話会

Monday 3rd, February 2020
14:00–15:00
Collaboration Room at 3F, Physics Department Bldg.

Unifying M_2AC Nanolamellar Carbides Under A Rigid Band Model Description

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The $M_{n+1}AX_n$, or "MAX" phases, where M is an early transition metal, A belongs to group 13-16 and X is C or N, are a class of nano-layered compounds that triggered strong interest from the material science community for their unique combinations of metal-like and ceramic-like properties [1]. They are also precursors for MXENES, a whole family of two-dimensional carbides [2], notably sought for energy storage developments [3]. Despite MAX phases attractiveness regarding a wide range of applications, some of their fundamental features are yet to be fully understood [4,6].

In this talk we propose a rigid band model that describes the electronic structure of all M_2AC, or "211" MAX phases [7,8]. Its applicability was confirmed by comparing predictions of density functional theory (DFT) to angle-resolved photoemission spectroscopy (ARPES) measurements performed on MAX phase single crystals. In V_2AlC, and in addition to conventional metallic bands, a nodal line and other linear band crossing features are found.

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[2] M. Naguib *et al.*, *Adv. Mater*. **23**, 4248 (2011).

[3] B. Anasori, M.R. Lukatskaya and Y. Gogotsi, *Nature Review Materials* **2**, 16098 (2017).

[4] T. Ouisse, L. Shi, B.A. Piot, B. Hackens, V. Mauchamp and D. Chaussende, *Phys. Rev. B* **92**, 045133 (2015).

[5] T. Ito, D. Pinek, T. Fujita, M. Nakatake, S. Ideta, K. Tanaka, T. Ouisse, *Physical Review B* **96** (19), 195168.

[6] D. Pinek, T. Ito, M. Ikemoto, M. Nakatake, T. Ouisse, *Physical Review B* **98** (3), 035120.

[7] M. H. Cohen and V. Heine, *Adv. Phys*. **7**, 395 (1958).

[8] D. Pinek, T. Ito *et al.*, *Phys. Rev. B* **100**, 075114 (2019).

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