

Orbital Selective Fermi Surface Shifts in Correlated AFeAs (A = Li, Na)

Geunsik Lee^{6*}, Hyo Seok Ji¹, Yeongkwan Kim², Changyoung Kim²,
Kristjan Haule³, Gabriel Kotliar³, Bumsung Lee⁴, Seunghyun Khim⁴,
Kee Hoon Kim⁴, Kwang S. Kim^{1,6}, Ki-Seok Kim⁵, Ji Hoon Shim^{1,5}

¹Department of Chemistry, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea

²Institute of Physics and Applied Physics, Yonsei University, Seoul, Republic of Korea

³Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

⁴Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea

⁵Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea

⁶Department of Chemistry, School of Natural Sciences UNIST (Ulsan National Institute of Science and Technology), Korea

E-mail: gslee@unist.ac.kr

Based on the dynamical mean field theory and angle resolved photoemission spectroscopy, we have investigated the mechanism of high T_c superconductivity in stoichiometric LiFeAs. The calculated spectrum is in excellent agreement with the observed angle resolved photoemission spectroscopy measurement. The Fermi surface (FS) nesting, which is predicted in the conventional density functional theory method, is suppressed due to the orbital-dependent correlation effect within the dynamical mean field theory method. We have shown that such marginal breakdown of the FS nesting is an essential condition to the spin-fluctuation mediated superconductivity, while the good FS nesting in NaFeAs induces a spin density wave ground state. Our results indicate that a fully charge self-consistent description of the correlation effect is crucial in the description of the FS nesting-driven instabilities.

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References

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