

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Sorting Category: 05.17.1 (T)

**Momentum density, Fermi surface and directional
Compton profile in the Iron-based superconductor LaOFeAs**

Y. J. WANG, HSIN LIN, B. BARBIELLINI, Northeastern U., P.E. MIJNARENDS, Northeastern U. and U. Tech., Delft, The Netherlands, S. KAPRZYK, Northeastern U. and Academy of Mining and Metallurgy AGH, Poland, W. AL-SAWAI, R.S. MARKIEWICZ, A. BANSIL, Northeastern U. — We have carried out first principles all-electron calculations of the (001) projected 2D electron momentum density (2D-EMD) and directional Compton profiles (CPs) along the [100], [001], and [110] directions in iron-based superconductor $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$ for various doping concentrations x within the framework of the local density approximation (LDA). We have identified Fermi surface features both in the 2D-EMD and in the CPs. Bonding effects related to the character of wave functions near the Fermi level are revealed by the autocorrelation function $B(r)$ defined as the Fourier transform of the momentum density. Work supported in part by the US Department of Energy.

Prefer Oral Session
 Prefer Poster Session

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Date submitted: 19 Nov 2008

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