



FIG. 5: (Color online) Temperature dependence of the EDC taken at $k_x = 0.52 \text{ \AA}^{-1}$. The inset is an enlargement of the top part of the spectra taken near the structural transition temperature.

existence of a short-ranged electronic ordering that locally doubles the unit cell, which can be captured by fast probes like ARPES. Because the evolution of band folding is smooth and no additional feature presents at the magnetic transition temperature, we can conclude that the short-ranged magnetic ordering must have developed at T_S . We note that elastic neutron scattering would not detect such magnetic domains due to cancellation of the scattering from anti-phase domains. Furthermore, recent muon spin resonance (μ SR) studies of NaFeAs could only detect SDW below T_N [18], indicating the fluctuation time scale of the magnetic domains are faster than the μ SR time scale above T_N .

The intimate relation between the electronic structure reconstruction and the structural/magnetic orderings is most remarkably represented by the fact that T_S is not only the onset of lattice distortion, but also the onset of the fluctuating SDW (as evidenced by the band folding) and electronic structure transition (the band shift). Our results clearly show that it is the electronic structure reconstruction that saves the total electronic energy significantly during both transitions. It is thus the driving force behind the magnetic transition and the rather soft structural transition (either through the SDW fluc-

tuations or directly). In parallel, Fermi surface nesting can be ruled out as the driving force for the SDW in NaFeAs for two primary reasons. First, it is clear that the band reconstruction goes beyond the nested (or semi-nested) portion of the Fermi surfaces near Γ and M . In fact, Fig. 3 shows that most of the bands, including the band far below the Fermi energy, participate in the reconstruction. Second, no gap has been observed at the Fermi crossings.

The reconstruction of the band structure here shares many common aspects with that in the “122” series of iron pnictides [20–22]. The scale of the shift, ordered moment, structural transition amplitude, and ordering temperature all roughly scale with each other in these compounds. Therefore, the band reconstruction scenario discussed here is most likely universal for the structural and magnetic transitions in all iron pnictides.

Models based on local magnetic exchange have successfully explained the subsequent transitions of lattice and magnetism, and they suggest that the lattice transition is driven by magnetic fluctuations [4, 23]. Moreover, local exchange interactions have been suggested to explain the observed band reconstruction, and they do have similar energy scales [20–22]. While our result can be viewed as a positive support of this picture, it also emphasizes that the electronic structure has to be taken into account in order to fully understand the transitions.

To summarize, we have carried out a systematic photoemission investigation of high quality NaFeAs single crystals, revealing the detailed electronic structure of the “111” series of iron pnictides for the first time. We show that the band structure undergoes significant shifts, and short-ranged magnetic ordering has already developed at the structural transition temperature. Our results suggest that electronic structure reconstruction, rather than Fermi surface nesting, plays a dominating role in causing both the lattice and magnetic transitions in iron pnictides, and support the existence of strong electron-electron correlation in these materials.

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- [1] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, *J. Am. Chem. Soc.* **130**, 3296 (2008).
 - [2] X. H. Chen *et al.*, *Nature (London)* **453**, 761 (2008).
 - [3] Z. A. Ren *et al.*, *Chin. Phys. Lett.* **25**, 2215 (2008).
 - [4] C. Fang *et al.*, *Phys. Rev. B* **77**, 224509 (2008).
 - [5] R. H. Liu *et al.*, *Nature (London)* **459**, 64 (2009).
 - [6] Q. Huang *et al.*, *Phys. Rev. Lett.* **101**, 257003 (2008).
 - [7] J. Zhao *et al.*, *Phys. Rev. B* **78**, 140504 (2008).
 - [8] W. Bao *et al.*, *Phys. Rev. Lett.* **102**, 247001 (2009).
 - [9] S. Li *et al.*, *Phys. Rev. B* **79**, 054503 (2008).
 - [10] C. de la Cruz *et al.*, *Nature (London)* **453**, 899 (2008).
 - [11] S. Li *et al.*, *Phys. Rev. B* **80**, 020504(R) (2009).
 - [12] D. H. Lu *et al.*, *Physica C* **469**, 452 (2009).
 - [13] G. F. Chen, W. Z. Hu, J. L. Luo, and N. L. Wang, *Phys. Rev. Lett.* **102**, 227004 (2009).
 - [14] H. Ding *et al.*, *Europhys. Lett.* **83**, 47001 (2008).
 - [15] H. Ding *et al.*, *New Journal of Physics* **11**, 025020 (2009).
 - [16] K. Kusakabe and A. Nakanishi, *J. Phys. Soc. Jpn.* **78**, 124712 (2009).
 - [17] F. Chen *et al.*, arXiv:1001.0855 [*Phys. Rev. B* (in press)].
 - [18] D. R. Parker *et al.*, arXiv:0909.0417 (unpublished).
 - [19] W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond* (Dover, New York, 1989).