

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Formation and suppression of Fe magnetism in ferropnictides

IGOR MAZIN, MICHELLE JOHANNES, Naval Research Laboratory — First, I will address the issue of how the Fe magnetic moment in HTC pnictides is formed in the DFT calculation, why is it so large (up to $2 \mu_B$) and why the moments prefer to order in a stripe-like AFM manner. The role of the onsite Hund rule coupling in forming the moment and the role of one-electron (band) energy in selecting an AFM pattern will be explained and emphasized. The important distinction between AFM interactions local in real space (superexchange, e.g. in cuprates) and local in momentum space (SDW or AFM in ferropnictides, which is *not* an SDW in spin-Peierls sense). This part will be largely based upon our preceding talk. Next, I will present some speculations about possible solitonic fluctuations (dynamic AFM domain boundaries) in this system, and their relations to experiments. This picture assumes that in the orthorhombic but nonmagnetic state the system consists of dynamic antiphase AFM domains, in the AFM state the domains are frozen (pinned), and in the nonmagnetic state dynamic twin domains dominate. This picture reconciles experiment, theory and first principle calculations in surprisingly many aspects.

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Date submitted: 21 Nov 2008

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