

Abstract Submitted  
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**Low-energy magnetic defects at nano- and meso-scale in Fe-based superconductors**<sup>1</sup> AFTAB ALAM, Department of Physics, Indian Institute of Technology Bombay, Powai, Mumbai 400076 Maharashtra, SUFFIAN N. KHAN, DUANE D. JOHNSON, Ames Laboratory, Ames, Iowa 500011, USA — In Fe-pnictides, "ordered" moments of Fe ( $0.8 - 1.04 \mu_B$ ) measured by neutron scattering in the antiferromagnetic groundstate are half ( $\sim 1.6 \mu_B$ ) of that estimated from density-functional theory (DFT), while other experiments are closer to DFT – a puzzle not yet understood. Structural and magnetic planar defects proliferate over differing length scales, and could be key to any moment description. Thus, we study via DFT the stability and magnetic properties of antiphase and domain boundaries, twins, and *nanotwins*, which exhibit low-moment states confined near defect boundaries. A single local-moment picture is thus inappropriate for long-range magnetic order. While the *nanoscale* defects are very low in energy, twins remain so at the mesoscale, where estimated distances between twin boundaries coincide with the observed magnetic correlation length. All these defects can be weakly mobile and/or have fluctuations that will lower assessed "ordered" moments from longer spatial and/or time averaging.

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