On the nature of an energy barrier between (π,0) and (0,π) magnetic orders in Fe pnictides

A. Yaresko, L. Boeri, and O.K. Andersen

Max Planck Institute for Solid State Research, Stuttgart, Germany

As temperature is lowered most of undoped Fe arsenides, parent compounds for recently discovered Fe based superconductors, undergo a transition into a collinear state with stripe-like magnetic order in which anti-ferromagnetic (AFM) Fe chains are ferromagnetically ordered along the direction perpendicular to the chains. Two such collinear magnetic structures, characterized by ordering vectors (π,0) or (0,π), are connected by infinite number of non-collinear states with two AFM sublattices of second Fe neighbors rotated by an arbitrary angle with respect to each other. In a classical Heisenberg model all these states are degenerate. Band structure calculation show, however, that the degeneracy is lifted already at the mean field LSDA level and that in Fe arsenides (π,0) and (0,π) magnetic orders are separated by an energy barrier comparable to the energy difference between Neel and stripe AFM orders. We discuss a microscopic origin of the energy barrier and demonstrate that it is caused by closely related to underlying band structure. The results for Fe arsenides are compared to $BaMn_2As_2$ and hypothetical KFe_2Se_2 for which we found that a non-collinear 90-degree spin arrangement is more favorable than collinear ones. A doping dependence of the barrier is also discussed.