MAR09-2008-005270

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

Competing Magnetic Interactions, Structural Phase Transition, and the Unprecedented Giant Coupling of Fe-spin State and the As-As Interactions in Iron-Pnictide

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From all-electron fixed-spin-moment calculations [1], we showed that the ferromagnetic and checkerboard antiferromagnetic ordering in LaOFeAs were not stable and the stripe Fe-spin configuration (i.e. SDW) was the only stable ground state. The main exchange interaction between Fe ions are large, antiferromagnetic, and frustrated. The magnetic stripe SDW phase breaks the tetragonal symmetry, removes the frustration, and causes a structural distortion. We unravel surprisingly strong interactions between arsenic ions, the strength of which is controlled by the Fe-spin state in an unprecedented way [2]. Reducing the Fe-magnetic moment, weakens the Fe-As bonding, and in turn, increases As-As interactions, causing giant reduction in the c-axis. For $CaFe_2As_2$ system, this reduction of c-axis with the loss of the Fe-moment is as large as 1.4 Å, an unheard of giant coupling of local spin-state of an ion to its lattice. Since the calculated large c-reduction has been recently observed only under high-pressure, our results suggest that the iron magnetic moment should be present in Fe-pnictides at all times at ambient pressure. Implications of these findings on the mechanism of superconductivity in iron-pnictides will be discussed.

[1] T. Yildirim, Phys. Rev. Lett. 101, 057010 (2008) (arXiv:0804.2252).
[2] T. Yildirim, arXiv:0807.3936 (2008)