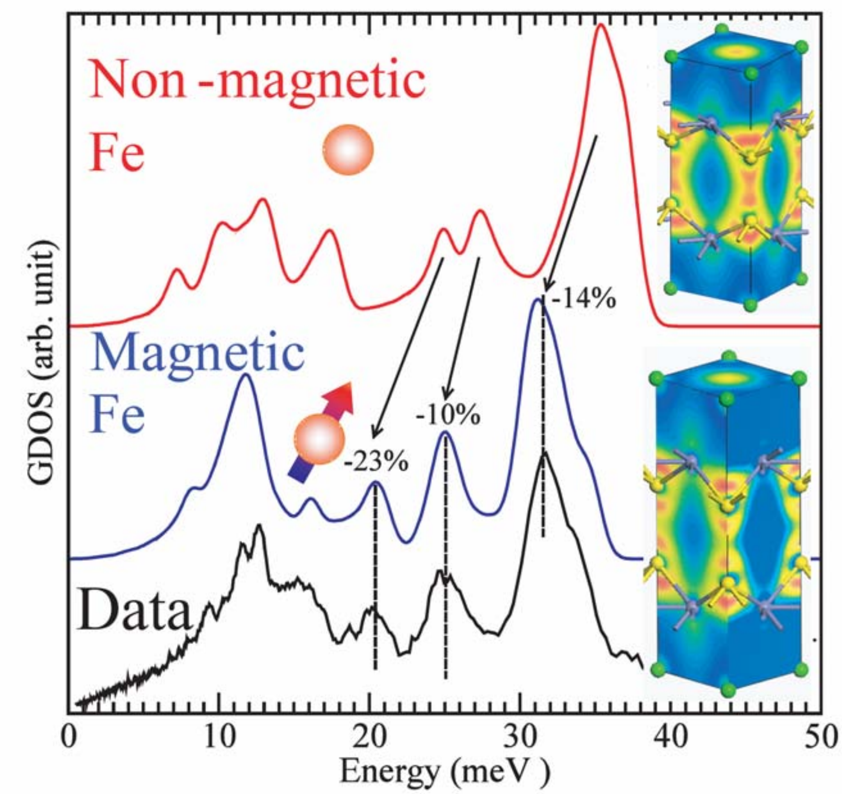
**Key Role of Iron-Spin in High-Temperature Iron-Arsenic Superconductors**




**Key Role of Iron-Magnetism in High-Temperature Fe-Pnictide Superconductors;** *Recent studies suggest that the Fe-spin is the key that controls atomic positions, lattice parameters, structural phase transition, phonons, and probably the superconductivity properties of these fascinating systems. See DETAILS…*

The figure shows comparisons of room temperature measured lattice vibration peaks (black) [4] in $BaFe_2As_2$ with theory in which the contribution of the iron spin is not accounted for (red), or is included (blue) which clearly gives much better agreement. In the insets the red areas show weaker bonding (bottom) to stronger (top) associated with shrinking in the $CaFe_2As_2$ system as the iron spin is turned off.

High-temperature superconductivity (high-Tc) discovered in 1986 remains one of the great, unexplained mysteries of condensed matter physics. The phenomenon was first found in a class of Cu-O-based compounds (cuprates). Although no explanation is yet completely satisfactory, the current belief is that the magnetic moments (i.e., spins) of the Cu ions play a major role in the superconductivity in these layered cuprates. Thus the situation has stood…until the recent discovery of an entirely new class of high-Tc superconductors featuring iron-arsenic (Fe-As) layers that are analogous to the Cu-O planes, the major structural feature in the cuprates. (As, arsenic, is a “pnictide”, hence these are called Fe-pnictide materials)

The key question now becomes: what is the mechanism of the superconductivity in these Fe-pnictide systems? The answer to this question is expected to shed light on the long-standing mystery of the mechanism of high-Tc superconductors in general. Once we have such an understanding of this phenomenon, we can make predictions and design new materials that superconduct at even higher temperatures and have more useful properties.

(The major current use of superconductivity is in cryogenically cooled electromagnets powering MRI machines.)

In his invited talk at the upcoming APS March meeting, NCNR's Taner Yildirim will present a brief review of his theory which clearly shows that the Fe-spin is the key factor controlling many physical properties of the pnictide systems, including atomic positions, crystal cell size, structural phase transitions, and lattice vibrations…and which provides a strong clue about the superconducting mechanism. Several examples will be presented which demonstrate that almost all of the observed structural and dynamical properties of Fe-pnictides can be explained in detail…provided that the Fe-spin be included in the calculations. In particular, he shows that giant magneto-elastic coupling (i.e., a large response of structure to a small change in the magnetization of its atoms) arises, and suggests that this enormous sensitivity of the structure to the Fe-spin may be the key ingredient in the mechanism of high-Tc superconductivity in Fe-pnictides.

**DETAILS**

From accurate quantum mechanics calculations Yildirim shows that there are strong and competing magnetic interactions in these systems that explain both the observed spin-pattern and the structural phase transition. His theory [1] predicted the sign of the lattice distortion which was later confirmed experimentally. Similarly, his prediction of very large magnetic exchange interactions (i.e., $J_1$ and $J_2$) has recently been confirmed by measurements of spin-waves up to 120 meV, which is almost the same energy scale as spin-waves in the cuprates.

When the iron magnetism is ignored, the calculations explain neither structure nor lattice vibration energies (i.e., phonons), resulting in large discrepancies between theory and experiment. In particular, he shows that when the Fe-spin is turned off [2], the system collapses, resulting for the case of $CaFe_2As_2$ in a 12 % reduction in the distance between Fe-As layers. The response of lattice size to the change in magnetic moment of its atoms is called magneto-elastic coupling and its magnitude is usually tiny, hardly measurable by x-ray or neutron scattering. However for the case of Fe-pnictide, this effect is enormous. To the best of our knowledge, such a giant coupling of the lattice to its atom-spin state has not been seen before.

In his work [2], Yildirim explains this unusual behavior by noting that As-As interaction is actually controlled by the Fe-As interaction which in turn is controlled by the Fe-spin state. When the Fe is non-magnetic, its interaction with the surrounding As ions is weaker, and therefore As turns its attention to the other As ions nearby, basically forming As-As bonds between adjacent planes. This causes the aforementioned 12 % shrinkage between planes. As shown in the figure above, Yildirim's theory [3] accurately predicts the positions of the measured lattice vibration peaks, which were incorrectly predicted by theories ignoring the Fe-spin contribution to the atomic forces. Turning on the Fe-spin softens two particular phonon modes (namely, As-atoms vibrating along a line between planes, and in-plane Fe-Fe stretching modes), as observed experimentally, and therefore, through fluctuations of the Fe-spin state, these modes could have very large effect on electronic structure. This effect may be related to the observed high-Tc. Yildirim is currently investigating this possibility.

More information may be obtained at Dr. Yildirim's website:
http://www.ncnr.nist.gov/staff/taner/highlights.htm

References:

1. *"Frustrated Magnetic Interactions, Giant Magneto-Elastic Coupling, and Magnetic Phonons in Iron-Pnictides"*, Taner Yildirim, Physica C, special issue on Fe-pnictides, in press (also arXiv:0902.3462 (2009)).

2. *"Strong Coupling of the Fe-Spin State and the As-As Hybridization in Iron-Pnictide Superconductors from First-Principle Calculations"*, Taner Yildirim, Phys. Rev. Lett. **102**, 037003 (2009).

3. *"Origin of the 150 K Anomaly in LaFeAsO: Competing Antiferromagnetic Interactions, Frustration, and a Structural Phase Transition"*, Taner Yildirim, Phys. Rev. Lett. **101**, 057010 (2008).

4. M. Zbiri, H. Schober, M.R. Johnson, S. Rols, R. Mittal, Y. Su, M. Rotter, D. Johrendt, Phys. Rev. B **29**, 064511 (2009).