

Pressure Effects on the Crystal Structure and Electronic Properties of the 1111 Iron Superconductors

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The study of the pressure effects on the crystal and electronic structure is a powerful tool that helps to find clues to analyze the superconducting state. The new iron based superconductors is an excellent example, where there are still plenty of opened questions to be answered.

In this presentation, we will discuss the effect of structural parameters under pressure on the superconducting properties on compounds belonging to 1111 Fe based family. In particular, we have observed a strong correlation of the crystal structure parameters on the T_C in (La,Sm)FeAsO_{1-x}F_x, LiFeAs compounds [1,2,3]. We have analyzed in detail the pressure dependence of the inter(intra)layer distance, the angle Fe-As-Fe and its effect on the T_C . These results are of great importance for band structure calculations based on realistic atomic positions that permit to obtain a detailed microscopic interpretation of the subtle effects on the electronic properties, explaining the effects on the superconducting transition. We also studied the pressure evolution of the structural and spin density wave transition in the SmFeAsO compound and we will correlate it with the superconducting properties.

[1] G. Garbarino et al, Phys Rev B (R) 2008, **78**, 100507

[2] G. Garbarino et al, sent to be published to PRB

[3] M. Mito, M. Pitcher, W. Crichton, G. Garbarino et al, J. Am. Chem. Soc, 2009, **131**, 2986