Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Orbital differentiation and the role of orbital ordering in the magnetic state of Fe superconductors ELENA BASCONES, BELEN VALENZUELA, MARIA J. CALDERON, Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, ICMM-CSIC (Spain) — There is increasing evidence for orbital differentiation and a possible coexistence of itinerant and localized electrons in Fe superconductors. In order to shed light on the role of the different orbitals on the magnetic state of these superconductors we analyze the metallic $(\pi, 0)$ antiferromagnetic state as a function of the interactions treated within mean field. We find that with increasing interactions the system does not evolve trivially from the pure itinerant to the pure localized regime. Instead we find a region with a strong orbital differentiation between xy and yz, which are half-filled gapped states at the Fermi level, and itinerant zx, $3z^2 - r^2$ and $x^2 - y^2$. We argue that orbital ordering between the yz and zx orbitals arises as a consequence of the interplay of the exchange energy in the antiferromagnetic x direction and the kinetic energy gained by the itinerant orbitals along the ferromagnetic y direction with an overall dominance of the kinetic energy gain. We indicate that iron superconductors may be close to the boundary between the itinerant and the orbital differentiated regimes and that it could be possible to cross this boundary with doping [arXiv: 1208.1917. Phys. Rev. B, November 2012].

Elena Bascones
Instituto de Ciencia de Materiales de Madrid,
Consejo Superior de Investigaciones Científicas, ICMM-CSIC

Date submitted: 19 Dec 2012 Electronic form version 1.4