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Ferro-Orbital Order and Anisotropic Magnetic Structure in Parent Compounds of Iron Pnictides CHI-CHENG LEE, WEI-GUO YIN, WEI KU, Brookhaven National Laboratory — Recently observed strong anisotropy of magnetic excitations [1] imposes a serious challenge to the current understanding of the electronic structure of parent compounds of iron pnictides. Here we examine the electronic structure of the representative LaOFeAs, using a first-principles Wannier-function analysis [2]. Without resorting to the widely employed frustration or nesting picture, a robust ferro-orbital ordering is found to give rise to the observed strongly anisotropic magnetic coupling, and drive both magnetic and lattice phase transitions. The revealed necessity of the additional orbital physics leads to a correlated electronic structure fundamentally distinct from that of the cuprates. In particular, the strong coupling to the magnons advocates the active roles of light orbitons in spin dynamics and electron pairing in iron pnictides.

[1] Jun Zhao et. al., Nature Physics, 5, 555 (2009)
[2] Chi-Cheng Lee et. al., http://arxiv.org/abs/0905.2957

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