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Electron delocalization, orbital order, magnetism, and emergent superconductivity in Fe_{1+y} Te and Fe_{1+y} (Te,S/Se)

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Neutron scattering [1] reveales an unusual enhancement, on warming, of dynamical magnetism in iron telluride, $Fe_{1+y}Te$, the non-superconducting parent material of the chalcogenide family of iron-based superconductors, and in nearly critical $Fe_{1+y}Te_{1-x}(S,Se)_x$, where bulk measurements show the presence of filamentary superconductivity [2]. While these findings are consistent with both Kondo-like screening of local spins by conduction electrons, or a delocalization, on cooling, of one of the electrons, our more recent results shed light on this issue, favoring the latter scenario. Investigation of the magnetostructural phase diagram of the $Fe_{1+y}Te$ series revealed that the low-temperature phase, which in the nearly stoichiometric ($y \approx 0$) material is attained via the first order phase transition at $T_N \approx 70$ K, is characterized not only by antiferromagnetic and structural order, but also by a peculiar type of orbital order. By combining results of bulk characterization of electronic behavior and the diffraction data on the microscopic structural changes for samples with $y \approx 0.05$ to 0.13, we were able to disentangle different low-temperature orders and identify new, electronically driven ferro-orbital ordering transition. The newly discovered orbital ordering is characterized by the formation of zigzag Fe-Fe chains similar to those in manganites, and is associated with the delocalization of one of the electrons. This has profound effect on magnetic and electronic properties, including marked decrease of resistivity and magnetic susceptibility.

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