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Microscopic origin of the structural and magnetic transitions in ferropnictide superconductor parent compounds MICHELLE JOHANNES, IGOR MAZIN, DEVINA PILLAY, Naval Research Laboratory — The parent ferropnictide compounds exhibit two transitions: one is an orthorhombic distortion and the other is a magnetic transition. The transitions are simultaneous in the 122 structural type, but the structural transition precedes the magnetic one in the 1111 type. Although this temperature separation implies that the magnetism depends on the distortion, our computational results show that exactly the opposite is true. The structural distortion is fully dependent on the existence of magnetism and will not occur if a magnetic moment is not present. The particularities of the distortion, namely the expansion along the axis containing aligned spins, occurs as a result of minimizing the one-electron (band) energies. We show that the distortion depends not only on the existence of a magnetic moment, but on the particular ordering pattern chosen by the spins. Imposing a checkerboard ordering results in full x/y symmetry, while a so-called stripe ordering results in near perfect agreement with experimental neutron data below the transition temperature. Our results indicate that, even in the doped (superconducting) compounds, the underlying physics is magnetic.

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