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Structural, spin, and orbital phase transitions in LaOFeAs: II. Wannier function analysis WEI-GUO YIN, CHI-CHENG LEE, WEI KU, Brookhaven National Laboratory — A realistic low-energy effective interacting Hamiltonian of doped LaOFeAs is derived quantitatively from a novel first-principles Wannier function analysis. Strong local orbital, spin, and lattice coupling to the doped charge is found associated with the orbital degree of freedom, which suggests a possible explanation of the high transition temperature. The fluctuations in the orbital sector fundamentally distinguish the iron pnictides from the copper oxide superconductors, and ensure the essential role of phonons in the mechanism of superconductivity in this new class of materials, in addition to electronic origin.

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