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Understanding the Origin of Magnetism in Various Iron-based Superconductors from Itinerant Limit YU-ZHONG ZHANG, MING-CUI DING, Tongji University, HAI-QING LIN, Beijing computational science research center — By investigating the bare susceptibilities from first principles which quantify the tendency of itinerant electrons towards magnetically ordered states, we find that the physical properties of various iron-based superconductors can be well understood by the relative strength of the particle-hole excitations at (π,π). Though the excitations in a few compounds show anomalous behaviors, they are not the counterexamples against the itinerant scenario. As long as the orbital degrees of freedom, which may lead to competing tendencies towards different magnetically ordered states, and the interlayer couplings are taken into account, these anomalies can be naturally accounted for from the itinerant limit. Moreover, we find that the particle-hole excitations away from the Fermi level are more relevant to the physical properties of iron-based superconductors than those close to the Fermi surfaces, which resolves the long-standing problem of why the Fermi surfaces alone can hardly explain various magnetic states observed experimentally in different iron-based superconductors. Finally, We predict based on our first principles calculations that K-doped $BaFe_2P_2$ and La- or Al-doped MgFeGe may be a possible iron-based superconductor.

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