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Hidden (π,0) instability as an itinerant origin of bicollinear antiferromagnetism in $Fe_{1+x}Te$[1] YU-ZHONG ZHANG, MING-CUI DING, School of physics science and engineering, Tongji University, Shanghai 200092, China, HAI-QING LIN, Beijing computational science research center, Beijing, China — By calculating orbitally resolved Pauli susceptibilities within maximally localized Wannier orbital basis transformed from first principles band structures, we find that magnetism in $Fe_{1+x}Te$ still has its itinerant origin even without Fermi surface nesting, provide orbital modulation of particle-hole excitations are considered. This leads to strong magnetic instabilities at wave vector (π,0)/(0,π) in d_{xz}/d_{yz} orbitals that are responsible for bicollinear antiferromagnetic state as extra electrons donated from excess Fe are considered. Magnetic exchange coupling between excess Fe and in-plane Fe further stabilizes the bicollinear antiferromagnetic order. Our results reveal that magnetism and superconductivity in iron chalcogenides may have different orbital origin, as Pauli susceptibilities of different orbitals evolves differently as a function of concentration of excess Fe and height of chalcogen atom measured from iron plane.

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Yu-Zhong Zhang
Tongji University, Shanghai, China

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