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Collinear (Bi-collinear) antiferromagnetic order in iron-pnictides (chalcogenides)[1] ZHONG-YI LU, Department of Physics, Renmin University of China, Beijing 100872, China, FENGJIE MA, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China , TAO XIANG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — By the first-principles electronic structure calculations, we find that the ground state of the tetragonal α-FeTe is in a bi-collinear antiferromagnetic order, in which the Fe local moments ($\sim 2.5\mu_B$) align ferromagnetically along a diagonal direction and antiferromagnetically along the other diagonal direction on the Fe-Fe square lattice. This novel bi- collinear order results from the interplay among the nearest, the next nearest, and the next next nearest neighbor superexchange interactions, mediated by Te $5p$-band. In contrast, the ground state of the other iron pnictides or chalogenides is in a conventional collinear antiferromagnetic order, like LaFeAsO, resulting from the interplay between the nearest and the next-nearest neighbor superexchange antiferromagnetic interactions, bridged by As atoms. This finding sheds new light on the origin of magnetic ordering in Fe-based superconductors.

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