Collinear (Bi-collinear) antiferromagnetic order in iron-pnictides (chalcogenides)\textsuperscript{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 \(\alpha\)-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.

\textsuperscript{1}This work is partially supported by National Natural Science Foundation of China and by National Program for Basic Research of MOST, China.

Zhong-Yi Lu
Department of Physics, Renmin University of China, Beijing 100872, China

Date submitted: 02 Dec 2008

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