On the difference between the pyroxenes LiFeSi\textsubscript{2}O\textsubscript{6} and LiFeGe\textsubscript{2}O\textsubscript{6} in their magnetic structures and spin orientations\textsuperscript{1}

CHANGHOON LEE, JISOOK HONG, JI HOON SHIM, Pohang University of Science and Technology, MYUNG-HWAN WHANGBO, North Carolina State University — The clinopyroxenes LiFeSi\textsubscript{2}O\textsubscript{6} and LiFeGe\textsubscript{2}O\textsubscript{6}, crystallizing in a monoclinic space group P\textsubscript{2}\textsubscript{1}/c, are isostructural and isoelectronic. Their crystal structures are made up of zigzag chains of edge-sharing FeO\textsubscript{6} octahedra containing high-spin Fe\textsuperscript{3+} ions, which run along the c direction. Despite this structural similarity, the two have quite different magnetic structures and spin orientations. In LiFeSi\textsubscript{2}O\textsubscript{6} the Fe spins have a ferromagnetic coupling within the zigzag chains along c and such FM chains have an antiferromagnetic coupling along a. In contrast, in LiFeGe\textsubscript{2}O\textsubscript{6}, the spins have an AFM coupling within the zigzag chains along c and such FM chains have an \( \uparrow\uparrow\downarrow\downarrow \) coupling along a. In addition, the spin orientation is parallel to c in LiFeSi\textsubscript{2}O\textsubscript{6}, but is perpendicular to c in LiFeGe\textsubscript{2}O\textsubscript{6}. To explain these differences in the magnetic structure and spin orientation, we evaluated the spin exchange parameters by performing energy mapping analysis based on LDA+U and GGA+U calculations and also by evaluating the magnetocrystalline anisotropy energies in terms of GGA+U+SOC and LDA+U+SOC calculations. Our study show that the magnetic structures and spin orientations of LiFeSi\textsubscript{2}O\textsubscript{6} and LiFeGe\textsubscript{2}O\textsubscript{6} are better described by LDA+U and LDA+U+SOC calculations.

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Changhoon Lee
Pohang University of Science and Technology

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