Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Pyroxenes: A novel class of multiferroics[1] D.I. KHOMSKII, Koeln University, S. JODLAUK, P. BECKER, J. MYDOSH, TH. LORENZ, S.V. STRELTSOV, D.C. HEZEL, L. BOHATY — Pyroxenes with the general formula $AMSi_2O_6$(A - mono- or divalent metal, M = di- or trivalent metal) are shown to be a new class of multiferroic materials. In particular, we have found so far that $NaFeSi_2O_6$ becomes ferroelectric in a magnetically ordered state below 6 K. Similarly, magnetically driven ferroelectricity is also detected in the Li homologues, $LiFeSi_2O_6$ (T_C =18 K) and $LiCrSi_2O_6$ (T_C =11 K). In all these monoclinic systems the electric polarization can be strongly modified by magnetic fields. Measurements of magnetic susceptibility, pyroelectric current and dielectric constants (and their dependence on magnetic field) are performed using a natural crystal of aegirine ($NaFeSi_2O_6$) and synthetic crystals of $LiFeSi_2O_6$ and $LiCrSi_2O_6$ grown from melt solution. For $NaFeSi_2O_6$ a temperature versus magnetic field phase diagram is proposed. Exchange constants are computed on the basis of ab initio band structure calculations. The possibility of a spiral magnetic structure caused by frustration as origin of the multiferroic behaviour is discussed. We propose that other pyroxenes may also be multiferroic, and that the versatility of this family offers an exceptional opportunity to study general conditions for and mechanisms of magnetically driven ferroelectricity.

[1]J. Phys.: Condens. Matter 19, 432201 (2007).

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Date submitted: 23 Nov 2007 Electronic form version 1.4