Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Trends in spin exchange interactions and ferroelectric polarization in the orthorhombic $R\mathbf{MnO_3}$ series SILVIA PICOZZI, KUNIHIKO YAMAUCHI, CNR-INFM LAquila, Italy, BIPLAB SANYAL, Uppsala Univ., Uppsala, Sweden, FRANK FREIMUTH, STEFAN BLUGEL, Forschungszentrum Julich, Germany, ELBIO DAGOTTO, Oak Ridge Natl. Lab. and Univ. Tennessee, TN, USA — Recently, magnetic ferroelectricity induced by Heisenberg-type interactions has been theoretically predicted in E-type antiferromagnetic (AFM) $HoMnO_3$ [1]. In order to fully clarify this unconventional microscopic mechanism, we have studied the structural, magnetic and ferroelectric properties for the entire family of orthorhombic $R\mathrm{MnO_3}$ (R= rare earth ions), based on first-principles density functional calculations. The ferromagnetic exchange interaction between nearest-neighbor Mn sites decreases with the ionic radius of R (concomitantly with the in-plane Mn-O-Mn bond angle), whereas the anti-ferromagnetic next-nearest neighbor interaction stays rather constant in the series. The competition of these exchange interactions results in a complicated magnetic phase diagram. The decrease in the Mn-O-Mn angle also affects the hopping integrals between Mn ions (as determined from Wannier functions), so that the calculated electric polarization in E-type AFM $R\mathrm{MnO_3}$ is remarkably reduced throughout the rare earth series.

[1]S. Picozzi et al., Phys. Rev. Lett. (in press)

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Date submitted: 26 Nov 2007 Electronic form version 1.4