Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Polar Behavior in a Magnetic Oxide Via A-Site Size Disorder[1]
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Density functional calculations are used to test a new mechanism for ferroelectricity in magnetic perovskites based on A-site size disorder. Calculations of the structure and magnetic ordering of (La,Lu)$MnNiO_6$ show that this mechanism is effective for this material, which is predicted to be both polar (ferroelectric or relaxor) and ferromagnetic, depending on the Lu concentration.

[1]Work supported by DOE, DMS&E.

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Date submitted: 21 Nov 2007 Electronic form version 1.4