P16

Hydrostatic Pressure Enhanced Ferroelectric Polarization in *ABC* ferroelectrics

Shi Liu[1] and R. E. Cohen[1,2]

[1]Extreme Materials Initiative, Geophysical Laboratory, Carnegie Institution for Science, Washington DC 20015, USA

[2]Department of Earth and Environmental Sciences, Ludwig-Maximilians-Universität, Munich 80333, Germany

Abstract

The origin of ferroelectricity comes from the delicate balance between the long-range Coulomb interaction that favors the polar phase and the short-range repulsion that favors the nonpolar phase. In general, the ferroelectric polarization decreases with increasing hydrostatic pressure. First-principles density functional theory calculations are carried out to study the effect of hydrostatic pressure on the structural and electronic properties of hexagonal *ABC* semiconducting ferroelectrics. We find that the electric polarization of *ABC* ferroelectrics containing Li increases in magnitude as a hydrostatic pressure is applied (Figure 1). Origin of this anomalous behavior is discussed.

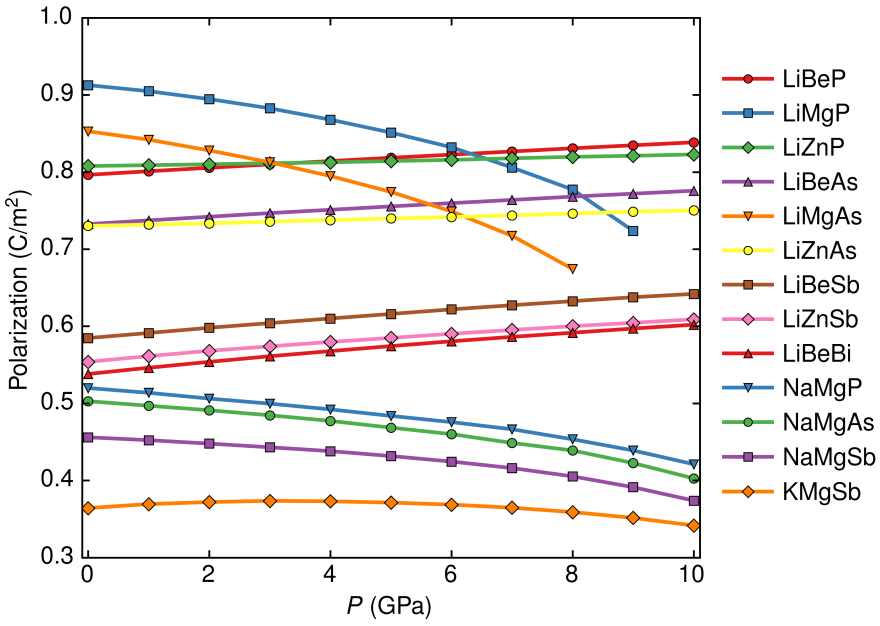

Figure 1. Polarization of *ABC* ferroelectrics as a function of hydrostatic pressure

Acknowledgments We thank the Carnegie Institution for Science, the US Office of Naval Research, and ERC Advanced Grant ToMCaT for support