$^{17}$O Nuclear Magnetic Resonance Chemical Shielding Calculations of PZT Solid Solutions\textsuperscript{1} DANIEL L. PECHKIS, ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — First principles B3LYP calculations of $^{17}$O NMR in PbTiO$_3$, Pb(Zr$_{1/2}$Ti$_{1/2}$)O$_3$ (PZT), and PbZrO$_3$ will be presented. These systems were modeled with finite size quantum clusters embedded in point charge arrays. The embedding reproduces the Ewald Coulomb potential to better simulate the crystal environment.\textsuperscript{3} For polar systems, the calculations were performed in the presence of an external electric field to cancel surface depolarization effects.\textsuperscript{4} PZT was modeled using three chemically ordered structures: P4mm, P2mm, and R3m. Two groupings of $^{17}$O isotropic chemical shifts $\delta_{\text{iso}}$ are seen in all of our PZT calculations with [001] ordering. One is at $\delta_{\text{iso}} \approx 400$ppm and the other is at $\delta_{\text{iso}} \approx 650$ppm. We relate these to variations in the Ti-O and Zr-O bond lengths and use this to interpret recent experimental measurements.\textsuperscript{5}

\textsuperscript{1}Supported by ONR
\textsuperscript{2}Supported by Virginia Space Grant Consortium Fellowship
\textsuperscript{4}S. Li and K. Rabe. APS March Meeting abstract (2007).