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Nuclear Magnetic Resonance Chemical Shift Calculation of Bulk Crystalline Materials[1] DANIEL PECHKIS, ERIC WALTER, HENRY KRAKAUER, College of William and Mary — Recent ^{17}O nuclear magnetic resonance (NMR) measurements for PZT solid solutions have given a new understanding of the local structure within this material. Due to the low signal to noise ratio in the experimental spectrum, some ambiguities in these data remain. The experimental results may be clarified by first principles density functional theory (DFT) calculations of the NMR properties. NMR is an excellent tool for studying short range chemical order in crystalline solid state systems. The electric field gradient experienced by quadrupole nuclei indicate the local symmetry of a crystallographic site. While the isotropic chemical shifts felt by the nuclei indicate the number of distinct crystallographic sites. The shift tensor shows the orientation of the nuclei with respect to the externally applied magnetic field. The tensor also indicates the variations in shielding by the electronic environment in response to an applied magnetic field. Our recent DFT ^{17}O chemical shift results of PZT will be presented.

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Daniel Pechkis
College of William and Mary

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