Abstract Submitted
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First-principles calculations of finite temperature Sc and O NMR parameters in $\mathbf{Pb(Sc_{2/3}W_{1/3})O_3}$[1] HENRY KRAKAUER, ERIC J. WALTER, JEREMY ELLDEN, GINA L. HOATSON, ROBERT L. VOLD, College of William and Mary — Understanding the dynamics of complex relaxor ferroelectrics is important to characterizing their large electromechanical coupling. Preliminary NMR measurements of Sc electric-field-gradients (EFG) in $Pb(Sc_{2/3}W_{1/3})O_3$ (PSW) show a strong temperature dependence in the range $T = 250 - 330$ K. To understand this behavior, we use the first-principles GIPAW[2] method within the Quantum Espresso (QE) package[3] to calculate ^{45}Sc and ^{17}O chemical-shifts and EFG tensors. To study finite temperature effects, we incorporate the thermal expansion of the lattice and sample thermal disorder, using the phonon degrees of freedom. As in our previous studies of perovksites,[4] we show that the ^{17}O chemical shifts in PSW also exhibit a linear correlation with the nearest-neighbor B-O bond length.

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[2]C. J. Pickard and F. Mauri, Phys. Rev. B **63**, 245101 (2001);
[3]P. Giannozzi et al., Journal of Physics: Condensed Matter **21**, 395502 (2009)
[4]D. L. Pechkis, E. J. Walter, and H. Krakauer. J. Chem. Phys. **135**, 114507 (2011); *ibid.* **131**, 184511 (2009)

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