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Electric Field Gradient Comparisons in Perovskites[1] DANDAN MAO, ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — Piezoelectric and dielectric properties of Pb-based complex ferroelectric alloys with the A(B'B"B"')O_3 perovskite structure depend on composition and the local ordering of the B-site cations. A prototypical example is $Pb(Sc_{1/2}Ta_{1/2})O_3$ (PST), which is a normal ferroelectric when the B atoms are ordered and becomes a relaxor when they are disordered. Electric field gradients (EFG) are sensitive to variations in local structure, and they can be probed using high-field nuclear magnetic resonance experiments. Calculations of EFGs are presented using the LAPW method within the local density approximation. We examine trends in B-site EFGs as a function of composition and order in PST, $Pb(Zr_{1-x}Ti_x)O_3$ (PZT), $Pb(Sc_{2/3}W_{1/3})O_3$ (PSW), and $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN). We discuss these results in terms of B- and Pb-atom off-centerings, and B-atom ordering.

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