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Eleectric Field Gradients and Born Effective Charges of PST DANDAN MAO, College of William and Mary, ERIC WALTER, College of William and Mary, HENRY KRAKAUER, College of William and Mary — Relaxor behavior in some complex ferroelectrics oxides is thought to be related to the local chemical environment. High magnetic field MAS NMR measurements have recently shown great promise as a microscopic probe of local structure of relaxors [1] by their ability to resolve electric field gradient (EFG) splittings. It is thus of considerable interest to be able to calculate EFGs in these materials. Here we present local density functional EFG calculations of $Pb(Sc\frac{1}{2}Ta\frac{1}{2})$ (PST) using the linear augmented planewave (LAPW) method. Our calculations focus on PST unit cells with different chemical ordering and ferroelectric phases. Trends of EFGs of PST and the correlation between EFGs and Born effective charges are discussed to better understand how local environments induce changes in EFGs.

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[1]G. Hoatson et al., *Phys. Rev. B* **66** 224103, (2002).

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