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Accurate calculations of the full NMR chemical shielding tensor in perovskites: B3LYP embedded cluster results for ^{17}O and ^{47,49}Ti[1]
DANIEL L. PECHKIS[2], ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — B3LYP calculations of ^{17}O and ^{47,49}Ti NMR in $BaTiO_3$ and $SrTiO_3$ will be presented. These systems were modeled with finite size quantum clusters embedded in classical fields generated from arrays of point charges and pseudopotentials. For polar clusters, an external E-field was applied to eliminate spurious depolarization fields. The full ^{17}O chemical shielding tensors, $\hat{\sigma}$(O), in $BaTiO_3$ and $SrTiO_3$ are in very good agreement with recent precise single crystal measurements.[3] The calculated Ti isotropic chemical shielding values are within the range of all reported measurements of $BaTiO_3$. Results will also be presented for the solid solution PZT series.

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[2]Supported by Virginia Space Grant Consortium Fellowship
[3]R. Blinc, et al., J. Phys: Cond. Matt. **20**, 085204 (2008).

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