Ab initio study of the relation between electric polarization and electric field gradients in ferroelectrics

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Electric Field Gradients can be used in a unique way to probe the polarization of materials when traditional methods cannot be applied. By using highly diluted concentrations, below ppm, of selected radioactive elements and isotopes to be combined with the Time Dependent Perturbed Angular Correlation technique, large amount of data becomes available that shows the applicability of the method for a large variety of materials.
In ferroelectric materials, the loss of inversion symmetry of the electronic charge distribution is necessary for the appearance of the electric polarization. On the other hand, the hyperfine interaction between the quadrupole moment of atomic nuclei and the electric field gradient (EFG) provides information on the electronic charge distribution close to a given atomic site. This suggests that measurements of hyperfine interactions may be exploited to study the ferroelectric order, which is especially interesting when standard techniques to measure polarization are not easily applied.
We present first-principles density functional theory calculations of ferroelectrics such as BaTiO3, KNbO3, PbTiO3 and other oxides with perovskite structures, by focusing on both EFG tensors and polarization. We analyze the EFG tensor properties such as orientation and correlation between components and their relation with electric polarization. This work supports previous studies of ferroelectric materials where a relation between EFG tensors and polarization was observed. This is an interesting possibility for the use of the perturbed angular correlation spectroscopy technique, which is ideal to study EFGs with varying conditions, with a large number of radioactive nuclei that can produced in specially designed targets.