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Ab-initio study of the correlation between electric field gradients and electric polarization in ferroelectric oxides

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The hyperfine interaction between the quadrupole moment of atomic nuclei and the electric field gradient (EFG) at the corresponding site provides information related to the near electronic charge distribution. Nuclear techniques such as Perturbed Angular Correlation (PAC) have been used to measure EFGs under temperature or electric field variations, for example, relating them to ferroelectric properties. Macroscopically, the main property in ferroelectrics is the polarization, which also depends on the charge density, but in many cases presents difficulties to be studied due to extrinsic effects. In previous hyperfine studies of ferroelectrics or multiferroics, particularly done at ISOLDE using PAC, a relation between the EFG and the polarization was observed and discussed in a few materials, but without a firm theoretical foundation.

We present first-principles density functional theory calculations for ferroelectric materials such as BaTiO3 , KNbO3 , PbTiO3, and other oxides with perovskite structures, with a simultaneous calculation and analysis of the two properties as a function of the ferroelectric distortion. The EFG tensor and its properties, including orientation, and correlation between components are examined. A relationship with the electric polarization is found, giving quantitative support to previous works.

The calculations allow a systematic study of this relationship in several compounds, which may help to relate more generally the conventional measurements of polarization and the local EFG experiments, and the added detailed information will potentially increase our understanding of the different mechanisms behind ferroelectrics or multiferroics.

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