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## APW+lo and TDPAC study of the Electric-Field Gradient at the cation sites of the $(^{44}\text{Ti}(\text{EC}) \rightarrow ^{44}\text{Sc})$ -doped $\text{Sc}_2\text{O}_3$ Semiconductor

We report on an ab-initio study of the Electric-Field-Gradient tensor (EFG) at both inequivalent Sc sites in the semiconductor  $\text{Sc}_2\text{O}_3$ . This semiconductor crystallizes in the bixbyite structure with two six-fold coordinated cation sites called C and D. The first is highly asymmetric whereas the second is axially symmetric. The calculations were performed applying the Full-Potential Augmented-Plane Waves plus local orbitals (FP-APW+lo) method, in the framework of the Density Functional Theory (DFT), that allows us to treat the electronic structure and the atomic structural position refinements in a fully self-consistent way. Our results are compared with experimental data determined by Time-Differential gamma-gamma Perturbed-Angular Correlation (TDPAC) spectroscopy using the Leipzig 6-detector TDPAC spectrometer with  $\text{LaBr}_3(\text{Ce})$  scintillators with the first excited  $I=1^-$  state of the  $^{44}\text{Ti}(\text{EC}) \rightarrow ^{44}\text{Sc}$  isotope as radioactive tracer. There is excellent agreement between experiment and the present ab-initio calculations. It is clear from the comparison of the experimental electric-field gradients and the Point-Charge Model (PCM) that the PCM can not describe even approximately the measured electric-field gradients at cation sites in pure scandium sesquioxide. In this simple situation, where the  $^{44}\text{Sc}$  probe atom is not an impurity in the material under study, the tracer does not introduce structural distortions that are usually not taken into account in the PCM when an impurity is concerned and that does not introduce impurity levels in the band gap of the semiconductor, which are usually critical for the origin of the electric-field gradient. Nevertheless, in this simple case, the PCM seems to fail. This can be only due to a poor description of the electronic distribution around the probe atom, which is not taken into account with the Sternheimer antishielding factor that is proposed in the PCM to describe the polarization of the core electrons of the probe atom. We also found an experimental site preference for the  $^{44}\text{Ti}$  impurity which can be understood by performing ab-initio calculations for the impurity system using super-cells.

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