FP-LAPW Study of the EFG at Impurity Sites in Oxides: Cd in Rutile TiO_2

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Z. Naturforsch. **55a,** 267–270 (2000); received August 26, 1999

Presented at the XVth International Symposium on Nuclear Quadrupole Interactions, Leipzig, Germany, July 25–30, 1999.

We report here first-principles determination of the electric-field gradient (EFG) tensor at the Cd impurity located at cation sites in rutile TiO_2. As far as we know, these represent the first *ab initio* calculations at impurity sites with the FP-LAPW method in oxide systems. We used super-cells to simulate the diluted impurity in the crystal. The free-relaxation process performed in our study shows that the changes in distances of the oxygen nearest-neighbours to the impurity are not isotropic as was supposed in a previous study within the muffin-tin approximation. Our prediction for the EFG component of major absolute value agrees well with the experiment and is opposite in sign and direction if isotropic relaxations are assumed. Our value of the asymmetry parameter η also compares very well with the experimental value.

Key words: Electric-Field Gradient; FP-LAPW; Impurity-Induced Lattice Relaxation; Electronic Structure; TiO_2.