

Erratum

L. A. Errico, G. Fabricius, and M. Rentería, FP-LAPW Study of the EFG at Impurity Sites in Oxides: Cd in Rutile TiO_2 , **55 a**, 267–270 (2000).

In Fig. 1 we have interchanged by mistake x and y axis. This does not alter the discussion of our calculations made in the paper, but 4th row in Table 1 (that refers to calculations of other authors) suffers the same interchange in xx and yy components of V_{ii} . Therefore, also the table and a sentence concerning comparison of both calculations have to be modified.

Corrected Figure 1:

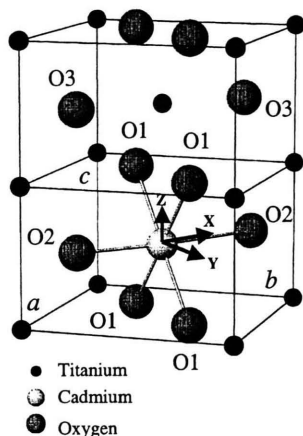


Fig. 1. Double super-cell used in the present work (see text). V_{ii} values throughout the article are referred to the principal axis system indicated in this figure.

Corrected Table 1:

Table 1. Experimental and theoretical electric-field gradients for Cd in TiO_2 in units of 10^{21} V/m^2 . The sign and directions of the experimental values are unknown. eq denotes the component of major absolute value.

	V_{XX}	V_{YY}	V_{ZZ}	eq	η
Experiment [13]				5.23 (5)	0.18 (1)
[14]				5.76 (2)	0.18 (1)
FP-LAPW					
Free-relaxation	-3.0	+5.0	-2.0	+5.0	0.2
Muffin-tin [5]					
Isotropic relax.	+3.56	+1.54	-5.09	-5.09	0.39
FP-LAPW					
Isotropic relax.	+3.6	+1.1	-4.7	-4.7	0.5

Corrected Paragraph of lines 7–12, 2nd column, page 270:

In this case we obtained very similar values for all the V_{ii} components of the EFG than they did (see Table 1), confirming that the different predictions made by the two approaches are due to the different relaxation proposed. The different methods employed to compute electronic structure produce no significant differences in the results.

