Erratum: Quantum-mechanical calculations of zircon to scheelite transition pathways in $ZrSiO_4$ [Phys. Rev. B 79, 104101 (2009)]

M. Flórez, J. Contreras-García, J. M. Recio, and M. Marqués

(Received 7 May 2009; published 27 May 2009)

DOI: 10.1103/PhysRevB.79.189903 PACS number(s): 61.50.Ks, 61.50.Ah, 64.60.A−, 81.30.Hd, 99.10.Cd

In Section III B, dedicated to the calculation of the atomic displacements along the pathways, an error occurred in the evaluation of the minimum displacement δ(O-O) from the $c/a=1.74$ ($\xi_{tet}=0.6446$) structure to the $c/a=1.78$ ($\xi_{tet}=0.6755$) structure of the tetragonal path. The value of δ(O-O) given in the second paragraph of this section (1.2145 Å) and also indicated in Fig. 3 (1.21 Å) should be replaced by 0.0466 Å. As a consequence, the correspondence between O atoms in these two structures changes: the correct minimum O-O displacement corresponds to the change of (x_O, y_O, z_O) from (0.1128, 0.4989, 0.2855) in the $c/a=1.74$ structure to (0.1201, 0.4963, 0.2881) and not to (−0.1201, 0.4963, 0.2881) as indicated in the text, in the $c/a=1.78$ structure. These latter are two crystallographic equivalent descriptions of the $c/a=1.78$ structure, with the same minimum O displacements with respect to the (0, 0.5653, 0.1946) description of the zircon structure, but not with respect to the (0.1128, 0.4989, 0.2855) description of the $c/a=1.74$ structure. The corrected value of the minimum O displacement in passing from $c/a=1.74$ to $c/a=1.78$ (0.0466 Å) is close to the difference of 0.0502 Å between $\delta_0(c/a=1.78)$ (1.0621 Å) and $\delta_0(c/a=1.74)$ (1.0119 Å), these δ_0 being the minimum displacements in passing from zircon to the $c/a=1.74$ and $c/a=1.78$ structures, respectively (see curve for the tetragonal path in Fig. 3). This result contrasts with the last statement in the third paragraph of Section III B.

The new correspondence between O atoms in the $c/a=1.74$ and $c/a=1.78$ structures removes the sharp increase (decrease) of the next-nearest (next-next-nearest) Zr-O distance at $c/a=1.74$ in passing from $c/a=1.74$ ($\xi_{tet}=0.6446$) to $c/a=1.78$ ($\xi_{tet}=0.6755$) shown in Fig. 4 and commented at the end of the second paragraph of Section III C. The corrected version of Fig. 4 is shown below.

The rest of results and conclusions of the paper remain unchanged.

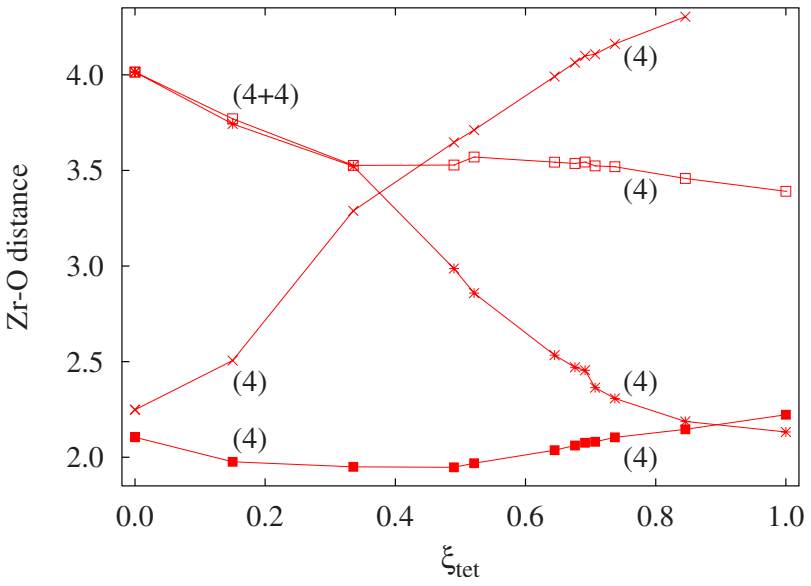

FIG. 1. (Color online) Corrected version of Fig. 4.

