Erratum


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

Corrected Figure 1:

![Double super-cell used in the present work (see text). $V_{eff}$ values throughout the article are referred to the principal axis system indicated in this figure.](image)

Corrected Table 1:

<table>
<thead>
<tr>
<th></th>
<th>$V_{xx}$</th>
<th>$V_{yy}$</th>
<th>$V_{zz}$</th>
<th>eq</th>
<th>$\eta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment [13]</td>
<td>5.23 (5)</td>
<td>0.18 (1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.76 (2)</td>
<td>0.18 (1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FP-LAPW Free-relaxation</td>
<td>-3.0</td>
<td>+5.0</td>
<td>-2.0</td>
<td>+5.0</td>
<td>0.2</td>
</tr>
<tr>
<td>Muffin-tin [5]</td>
<td>+3.56</td>
<td>+1.54</td>
<td>-5.09</td>
<td>-5.09</td>
<td>0.39</td>
</tr>
<tr>
<td>Isotropic relax.</td>
<td>+3.6</td>
<td>+1.1</td>
<td>-4.7</td>
<td>-4.7</td>
<td>0.5</td>
</tr>
<tr>
<td>FP-LAPW Isotropic relax.</td>
<td>+3.6</td>
<td>+1.1</td>
<td>-4.7</td>
<td>-4.7</td>
<td>0.5</td>
</tr>
</tbody>
</table>

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

In this case we obtained very similar values for all the $V_{eff}$ 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.