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Correction: A new computational strategy to calculate the edge energy of a relaxed step. Calcite (CaCO_3) as a case study

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Correction for 'A new computational strategy to calculate the edge energy of a relaxed step. Calcite (CaCO_3) as a case study' by M. Bruno et al., *CrystEngComm*, 2021, 23, 7340–7347, <https://doi.org/10.1039/D1CE01119G>.

The authors regret an error in the calculation of the values of the edge energies listed in Table 2: the calculations were performed without considering the factor of 2 in eqn (1). The correct Table 2 is shown below.

Table 2 Edge energy, ρ , of the $[\bar{4}41]$, $[4\bar{2}1]$ and $[010]$ steps running on the (10.4) face of calcite. Labels Ca and CO_3 indicate the termination of the step ledge

Step edges	ρ (J m^{-1})
Acute- $[\bar{4}41]$	8.10×10^{-11}
Obtuse- $[\bar{4}41]$	1.38×10^{-10}
$[4\bar{2}1]_{\text{Ca}}$	1.34×10^{-10}
$[4\bar{2}1]_{\text{CO}_3(\text{A})}$	3.22×10^{-10}
$[4\bar{2}1]_{\text{CO}_3(\text{B})}$	1.26×10^{-10}
Acute- $[010]_{\text{Ca}}$	1.34×10^{-10}
Obtuse- $[010]_{\text{Ca}}$	1.48×10^{-10}
Acute- $[010]_{\text{CO}_3}$	1.65×10^{-10}
Obtuse- $[010]_{\text{CO}_3}$	1.25×10^{-10}

Accordingly, the relaxed 2D equilibrium shape (ES) of the nucleus on the (10.4) face calculated with the edge energies in Table 2 and reported in Fig. 5 of the original paper is wrong. The correct Fig. 5 is shown below.

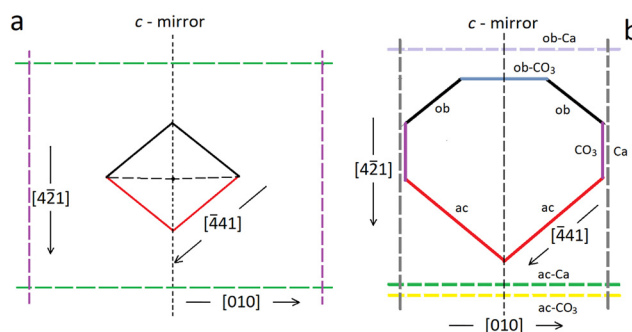


Fig. 5 (a) Unrelaxed and (b) relaxed 2D equilibrium shapes (ESs) of the nucleus on the (10.4) face. The arrows indicate the directions of the steps. Labels ac and ob represent the acute and obtuse steps, respectively, while Ca and CO_3 indicate the atomic step terminations. The quantitative comparison of the unrelaxed and relaxed ESs clearly shows the different sizes of the 2D nuclei and that, when relaxed, all the step energies are closer to each other. Owing to this property, the shape of the 2D nuclei should become more sensitive to the foreign adsorption (solvent, impurities) on the step ledges.

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This mistake also led to a misinterpretation of the literature data reported in several parts of the manuscript:

1. In the Abstract, the sentence “We calculated, as the most stable step, the acute $[\bar{4}41]$ edge ($\rho = 5.04 \times 10^{-10} \text{ J m}^{-1}$), followed by the Ca-terminated acute-[010] ($5.39 \times 10^{-10} \text{ J m}^{-1}$) and Ca-terminated $[\bar{4}21]$ ($9.77 \times 10^{-10} \text{ J m}^{-1}$)” must be replaced by “We calculated, as the most stable step, the acute $[\bar{4}41]$ ledge ($\rho = 8.10 \times 10^{-11} \text{ J m}^{-1}$), followed by the CO_3 -terminated obtuse-[010] ($1.25 \times 10^{-10} \text{ J m}^{-1}$) and CO_3 -terminated $[\bar{4}21]$ ($1.26 \times 10^{-10} \text{ J m}^{-1}$)”.

2. In section “3.1. Acute and obtuse $[\bar{4}41]$ steps on the (10.4) face”, the sentences “The edge energies of the acute- $[\bar{4}41]$ and obtuse- $[\bar{4}41]$ edges are 5.04×10^{-10} and $6.19 \times 10^{-10} \text{ J m}^{-1}$, respectively (Table 2). Kristensen *et al.*³ estimated the ρ values for acute- $[\bar{4}41]$ and obtuse- $[\bar{4}41]$ edges of 2.37×10^{-10} and 1.26×10^{-10} , respectively, which are noteworthy lower than ours. And on top of that, according to their calculations, the obtuse- $[\bar{4}41]$ edge is more stable than the acute- $[\bar{4}41]$ one, which is the opposite of that we obtained with our simulations. Nygren *et al.*¹⁵ calculated an average edge energy for the acute and obtuse steps of $2.5 \times 10^{-10} \text{ J m}^{-1}$, a value lower than our averaged step energy, $5.62 \times 10^{-10} \text{ J m}^{-1}$, and slightly higher with respect to that by Kristensen *et al.*,³ $1.82 \times 10^{-10} \text{ J m}^{-1}$ ” must be replaced by “The edge energies of the acute- $[\bar{4}41]$ and obtuse- $[\bar{4}41]$ edges are 8.10×10^{-11} and $1.38 \times 10^{-10} \text{ J m}^{-1}$, respectively (Table 2). Kristensen *et al.*³ estimated the ρ values for acute- $[\bar{4}41]$ and obtuse- $[\bar{4}41]$ edges of 2.37×10^{-10} and 1.26×10^{-10} , respectively. According to their calculations, the obtuse- $[\bar{4}41]$ edge is more stable than the acute- $[\bar{4}41]$ one, which is the opposite of that we obtained with our simulations. Nygren *et al.*¹⁵ calculated an average edge energy for the acute and obtuse steps of $2.5 \times 10^{-10} \text{ J m}^{-1}$, a value higher than our averaged step energy, $1.09 \times 10^{-10} \text{ J m}^{-1}$, and slightly higher with respect to that by Kristensen *et al.*,³ $1.82 \times 10^{-10} \text{ J m}^{-1}$ ”.

3. The discussion in points 1 and 2 on page 7345 (left column, rows 22–42) should be disregarded.

4. In section “3.2. $[\bar{4}21]$ steps on the (10.4) face”, the sentences “We only show in Fig. 3b the relaxed structure of the $[\bar{4}21]_{\text{Ca}}$ edge, since it has the lowest edge energy (Table 2), $9.77 \times 10^{-10} \text{ J m}^{-1}$. Nevertheless, this value is almost twice with respect to that of the acute- $[\bar{4}41]$ edge. The ρ values of the $[\bar{4}21]_{\text{CO}_3(\text{A})}$ and $[\bar{4}21]_{\text{CO}_3(\text{B})}$ edges are 1.30×10^{-9} and 2.57×10^{-9} , respectively. To the best of our knowledge, no experimental values exist to compare with our theoretical ones. There is only an unrelaxed average value calculated at the empirical level by Massaro *et al.*,²⁰ $15.80 \times 10^{-10} \text{ J m}^{-1}$, by using the same strategy described by Aquilano *et al.*,⁶ such a value is slightly lower than our averaged relaxed one, $16.16 \times 10^{-10} \text{ J m}^{-1}$ ” must be replaced by “We only show in Fig. 3b the relaxed structure of the $[\bar{4}21]_{\text{Ca}}$ edge, which has an edge energy of $1.34 \times 10^{-10} \text{ J m}^{-1}$ (Table 2). The ρ values of the $[\bar{4}21]_{\text{CO}_3(\text{A})}$ and $[\bar{4}21]_{\text{CO}_3(\text{B})}$ edges are 3.22×10^{-10} and $1.26 \times 10^{-10} \text{ J m}^{-1}$, respectively. To the best of our knowledge, no experimental values exist to compare with our theoretical ones. There is only an unrelaxed average value calculated at the empirical level by Massaro *et al.*,²⁰ $15.80 \times 10^{-10} \text{ J m}^{-1}$, by using the same strategy described by Aquilano *et al.*,⁶ such a value is higher than our averaged relaxed one, $1.94 \times 10^{-10} \text{ J m}^{-1}$ ”.

5. In section “3.3. Acute and obtuse [010] steps on the (10.4) face”, the sentences “According to the calculated edge energies (Table 2), the following stability order of the steps is obtained: acute-[010]_{Ca} < acute-[010]_{CO₃} < obtuse-[010]_{Ca} < obtuse-[010]_{CO₃}. The edge energy of the acute-[010]_{Ca} step is $5.39 \times 10^{-10} \text{ J m}^{-1}$, slightly higher than that of the most stable acute- $[\bar{4}41]$ step. Interestingly, the acute-[010] steps (both Ca and CO_3 -terminated) have edge energies lower than the obtuse ones, just like for the $[\bar{4}41]$ step. Also in this case, no experimental values of ρ exist to compare with our theoretical ones. There is only an unrelaxed average value calculated at the empirical level by Massaro *et al.*,²⁰ $11.43 \times 10^{-10} \text{ J m}^{-1}$, which is similar to the ρ value we obtained for the obtuse-[010]_{CO₃} edge (Table 2)” must be replaced by “According to the calculated edge energies (Table 2), the following stability order of the steps is obtained: obtuse-[010]_{CO₃} < acute-[010]_{Ca} < obtuse-[010]_{Ca} < acute-[010]_{CO₃}. The edge energy of the obtuse-[010]_{CO₃} step is $1.25 \times 10^{-10} \text{ J m}^{-1}$, slightly higher than that of the most stable acute- $[\bar{4}41]$ step. Also in this case, no experimental values of ρ exist to compare with our theoretical ones. There is only an unrelaxed average value calculated at the empirical level by Massaro *et al.*,²⁰ $11.43 \times 10^{-10} \text{ J m}^{-1}$ ”.

6. In section “4. Conclusions”, the sentence “In particular, we observed that the most stable is the acute- $[\bar{4}41]$ step with $\rho = 5.04 \times 10^{-10} \text{ J m}^{-1}$, followed by the Ca-terminated acute-[010] step ($5.39 \times 10^{-10} \text{ J m}^{-1}$) and Ca-terminated $[\bar{4}21]$ step ($9.77 \times 10^{-10} \text{ J m}^{-1}$)” must be replaced by “In particular, we observed that the most stable is the acute- $[\bar{4}41]$ step with $\rho = 8.10 \times 10^{-11} \text{ J m}^{-1}$, followed by the CO_3 -terminated obtuse-[010] ($1.25 \times 10^{-10} \text{ J m}^{-1}$) and CO_3 -terminated $[\bar{4}21]$ ($1.26 \times 10^{-10} \text{ J m}^{-1}$)”.

In section “4. Conclusions”, the sentences “2. The calculations in this work deeply change the situation: the acute-[010]_{Ca} step cuts the two $\langle \bar{4}41 \rangle$ steps linked by the glide symmetry plane, whereas this does not happen for the obtuse-[010]_{Ca} step (Fig. 5b). Both the acute- and obtuse-[010] steps with CO_3 termination never became a part of the ES. 3. The $\langle \bar{4}21 \rangle$ step with Ca termination does not (for very little) become a part of the ES, but it is highly probable that the adsorption of the solution on the step (certainly reducing the value of the edge energy) can bring this edge into play as well” must be replaced by “2. The calculations in this work deeply change the situation: the obtuse-[010]_{CO₃} step cuts the two $\langle \bar{4}41 \rangle$ steps linked by the glide symmetry plane, whereas this does not happen for the acute-[010]_{CO₃} step (Fig. 5b). Both the acute- and obtuse-[010] steps with Ca termination never become part of the ES. 3. The $\langle \bar{4}21 \rangle$ step with CO_3 termination becomes part of the ES”.

These errors do not affect the overall conclusions of the paper.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

