Erratum: Synthetic ferromagnetic nitrides: First-principles calculations of CaN and SrN [Phys. Rev. B 76, 054433 (2007)]

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In Fig. 4 of our paper, we plotted the enthalpies of 2CaN+Ca assuming the structure of Ca as fcc, bcc, or sc. When we evaluated the enthalpies using the equation,

$$H = 2H_{\mathrm{CaN}} + H_{\mathrm{Ca}} = 2(E_{\mathrm{CaN}} + p_{\mathrm{CaN}}V_{\mathrm{CaN}}) + (E_{\mathrm{Ca}} + p_{\mathrm{Ca}}V_{\mathrm{Ca}})$$

with the condition $p_{\mathrm{CaN}}=p_{\mathrm{Ca}}=p$, we mistakenly used incorrect data of p_{Ca}. When we corrected this error, we found that the enthalpy curves of β-Ca_3N_2 and 2CaN+Ca do not cross each other. The corrected Fig. 4 is shown below and this should replace the incorrect one in the paper.

As a result, the discussions related with this enthalpy crossing should be removed and the following corrections are necessary in the paper:

(i) In the abstract, the last sentence, "We propose a … temperature environment." should be removed.

(ii) In the "RESULTS AND DISCUSSION" section, the sentences from line 36 of the right-hand-side column on page 3

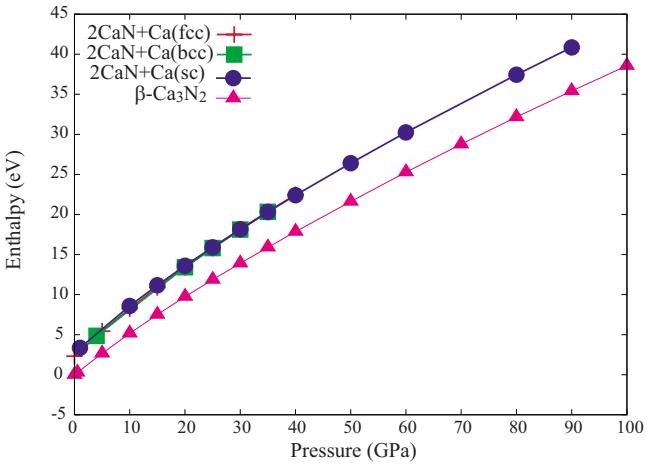

FIG. 4. (Color online) The enthalpy of β-Ca_3N_2 and the sum, 2CaN+Ca, as functions of pressure. Three types of structures of Ca are assumed and plotted.

(054433-3) to line 4 of the right-hand-side column on page 4 (054433-4) should be removed. (That part begins with "We now proceed to propose ideas for…" and ends with "…decompress it to ambient pressure.")

(iii) In the CONCLUSION section, the sentences from lines 17 to 19, beginning with "The process for synthesizing … of the first-principles calculations." should be removed.

All of the other results and conclusions presented in the paper remain unchanged.

One of the authors (M.G.) has successively investigated this material[1] and has studied the mechanical stability of this RS-CaN. The mechanical stability is controversial because the results depend on the selection of the exchange-correlation potential in the DFT calculations. This correction does not affect the magnetic properties.

[1] M. Geshi, Physica B **405**, 517 (2010).

