THE JOURNAL OF PHYSICAL CHEMISTRY C

ADDITION/CORRECTION

pubs.acs.org/JPCC

Correction to "Niobium Doping Effects on Performance of $BaCo_{0.7}Fe_{0.3-x}Nb_xO_{3-\delta}$ Perovskite" [*The Journal of Physical Chemistry C* **2010**, *114*, 22338–22345. DOI: 10.1021/jp108306z].

PeiJun Shen,* Xu Liu, HaiHai Wang, and WeiZhong Ding

Some errors were found in our simulating models. After we correct these errors, the consequences and the conclusions of the paper are still valid. However, there are a number of errors have to be corrected in our paper.

Figure 2 is corrected here.

Page 22342, first column, 16 lines down, the correct description should be "Because the ionic affinity with O has Nb > Fe > Co, statistically the oxygen farther away from dopants has the weaker binding to bulk, and the niobium doping raises the formation energy of oxygen vacancy in perovskite."

Page 22342, first column, 34 lines down, the correct description should be "The r_{rms} in the 1-, 2-, 3-, or 4-configuration of the $BaCo_{0.75}Fe_{0.125}Nb_{0.125}O_{3-\delta}$ model in Figure 9 is 0.157, 0.145, 0.160, or 0.144 Å, respectively; thus the lower formation energy

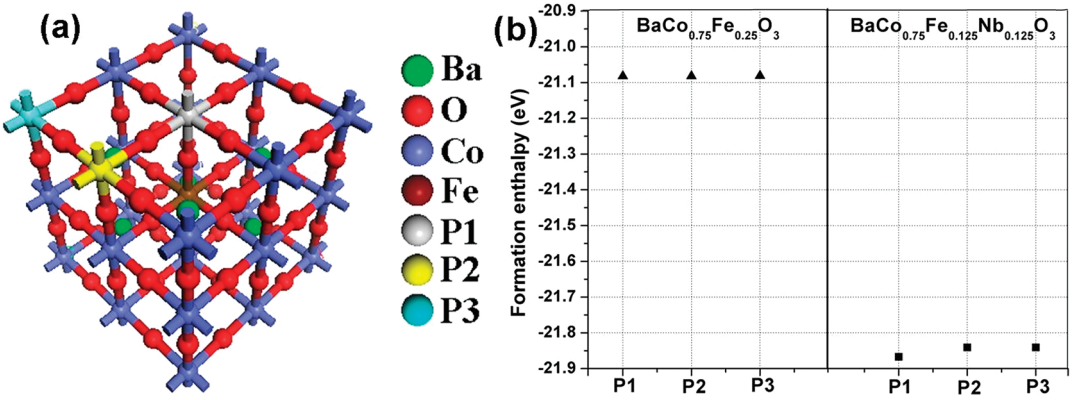

Figure 2. (a) Structure schematics of $BaCo_{0.75}M_{0.25}O_3$ supercells. (b) Calculated formation enthalpy for $BaCo_{0.75}Fe_{0.25}O_3$ and $BaCo_{0.75}Fe_{0.125}Nb_{0.125}O_3$ in which the second dopant (Fe or Nb) substitutes are at the P1, P2, or P3 position.

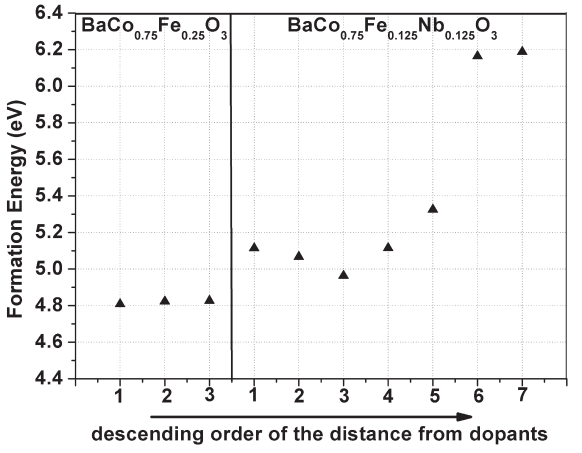

Figure 9. Formation energy for oxygen vacancies at different positions in $BaCo_{0.75}Fe_{0.25}O_3$(P3) and $BaCo_{0.75}Fe_{0.125}Nb_{0.125}O_3$(P1) models under oxygen-rich conditions.

Published: August 30, 2011

in 2- and 3-configurations cannot be attributed to the atomic relaxation around the vacancy."

Figure 9 is corrected here.

DOI: 10.1021/jp207657q
Published on Web ■■■