



Cite this: *Phys. Chem. Chem. Phys.*, 2016, **18**, 8242

DOI: 10.1039/c6cp90049f

www.rsc.org/pccp

## Correction: *Ab initio* and empirical defect modeling of $\text{LaMnO}_{3\pm\delta}$ for solid oxide fuel cell cathodes

Yueh-Lin Lee,<sup>†a</sup> Shenzhen Xu<sup>a</sup> and Dane Morgan<sup>\*ab</sup>

Correction for '*Ab initio* and empirical defect modeling of  $\text{LaMnO}_{3\pm\delta}$  for solid oxide fuel cell cathodes' by Yueh-Lin Lee et al., *Phys. Chem. Chem. Phys.*, 2012, **14**, 290–302.

The authors have identified two typos in the manuscript. These typos do not influence any calculation results in the paper but might be confusing for the reader. In Table 1, the second equation down from the header "Expression", the unit should be  $\text{eV}/(1000 \text{ K})^{-1}$  per  $\text{O}_2$  and the corrected equation should read:

$$S_{\text{O}_2}^{\text{NIST}} = A \times \ln(t) + B \times t + C \times \frac{t^2}{2} + D \times \frac{t^3}{3} - \frac{E}{2 \times t^2} + G, (\text{eV}(1000 \text{ K})^{-1}/\text{O}_2)$$

In Table 1, the fourth equation down from the header "Expression",  $T$  should be  $T_{\text{R}}$  and the corrected equation should read:

$$H_{\text{vib}}^0(\text{O}_{\text{solid}}^{2-}) = 3k_{\text{b}}T_{\text{R}} \cdot \left(\frac{\theta_{\text{E}}}{2T_{\text{R}}}\right) \cdot \coth\left(\frac{\theta_{\text{E}}}{2T_{\text{R}}}\right)$$

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

<sup>a</sup> Materials Science Program, 1509 University Avenue, Madison, Wisconsin, 53706-1595, USA

<sup>b</sup> Department of Materials Science and Engineering, 1509 University Avenue, Madison, Wisconsin, 53706-1595, USA. E-mail: ddmorgan@wisc.edu; Fax: +1 608-262-8353; Tel: +1 608-265-5879

<sup>†</sup> Current affiliation: National Energy Technology Laboratory, 626 Cochran Mill Road, P.O. Box 10940, Pittsburgh, PA 15236-0940, USA

