

Cite this: *J. Mater. Chem. A*, 2019, 7, 20438

## Correction: Interplay between H<sub>2</sub>O and CO<sub>2</sub> coadsorption and space-charge on Y-doped BaZrO<sub>3</sub> surfaces

Jonathan M. Polfus,<sup>a</sup> Jing Yang,<sup>b</sup> and Bilge Yildiz<sup>\*,bc</sup>

DOI: 10.1039/c9ta90210d

Correction for 'Interplay between H<sub>2</sub>O and CO<sub>2</sub> coadsorption and space-charge on Y-doped BaZrO<sub>3</sub> surfaces' by Jonathan M. Polfus *et al.*, *J. Mater. Chem. A*, 2018, 6, 24823–24830.

www.rsc.org/MaterialsA

The calculated entropies of H<sub>2</sub>O and CO<sub>2</sub> chemisorption presented in Table 2 in the published article,  $-6.37 \times 10^{-4}$  eV K<sup>-1</sup> and  $-8.78 \times 10^{-4}$  eV K<sup>-1</sup>, respectively, were not correct due to an error in the reference value used for gaseous H<sub>2</sub>O and CO<sub>2</sub>. The correct adsorption entropies are  $-1.39 \times 10^{-3}$  eV K<sup>-1</sup> for H<sub>2</sub>O and  $-1.68 \times 10^{-3}$  eV K<sup>-1</sup> for CO<sub>2</sub>, respectively.

The less favorable adsorption entropies lead to somewhat lower surface coverages, especially as the temperature increases (Fig. 4). Overall, surface protons become relatively more favored and predominate over carbonate adsorbates across a wider range of temperature and pressure. Hydroxide species become less relevant, and consequently, the maximum space-charge potential increases from about 0.3 V at 500–700 K to about 0.4 V at 500–600 K.

Fig. 7 illustrates that taking into account coadsorption and space-charge formation remains crucial for the calculated surface coverages. Despite the current numerical corrections, the overall findings and conclusions in the original manuscript remain the same.

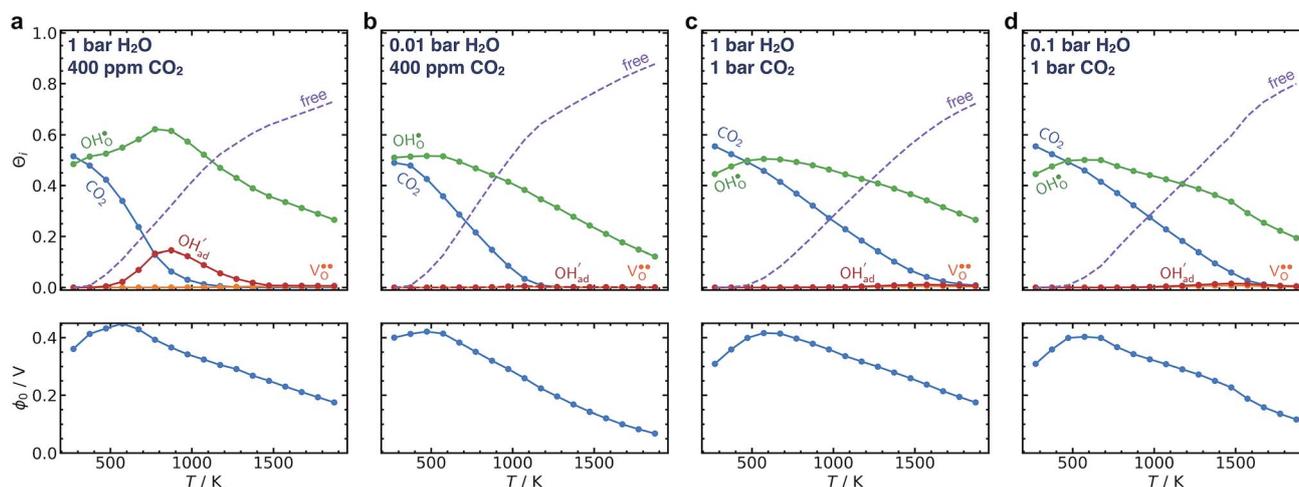


Fig. 4 Surface coverages of adsorbates and defects (protons, oxygen vacancies, hydroxide and carbonate species) as well as free surface sites (top) and the corresponding space-charge potential (bottom) on BaZr<sub>0.8</sub>Y<sub>0.2</sub>O<sub>3</sub> (0 0 1) as a function of temperature under 1 bar H<sub>2</sub>O, 400 ppm CO<sub>2</sub> (a), 0.01 bar H<sub>2</sub>O, 400 ppm CO<sub>2</sub> (b) and 1 bar CO<sub>2</sub>, 1 bar H<sub>2</sub>O (c) and 0.1 bar H<sub>2</sub>O, 1 bar CO<sub>2</sub>.

<sup>a</sup>SINTEF Industry, Sustainable Energy Technology, PO Box 124 Blindern, NO-0314 Oslo, Norway. E-mail: jonathan.polfus@sintef.no

<sup>b</sup>Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

<sup>c</sup>Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA. E-mail: byildiz@mit.edu



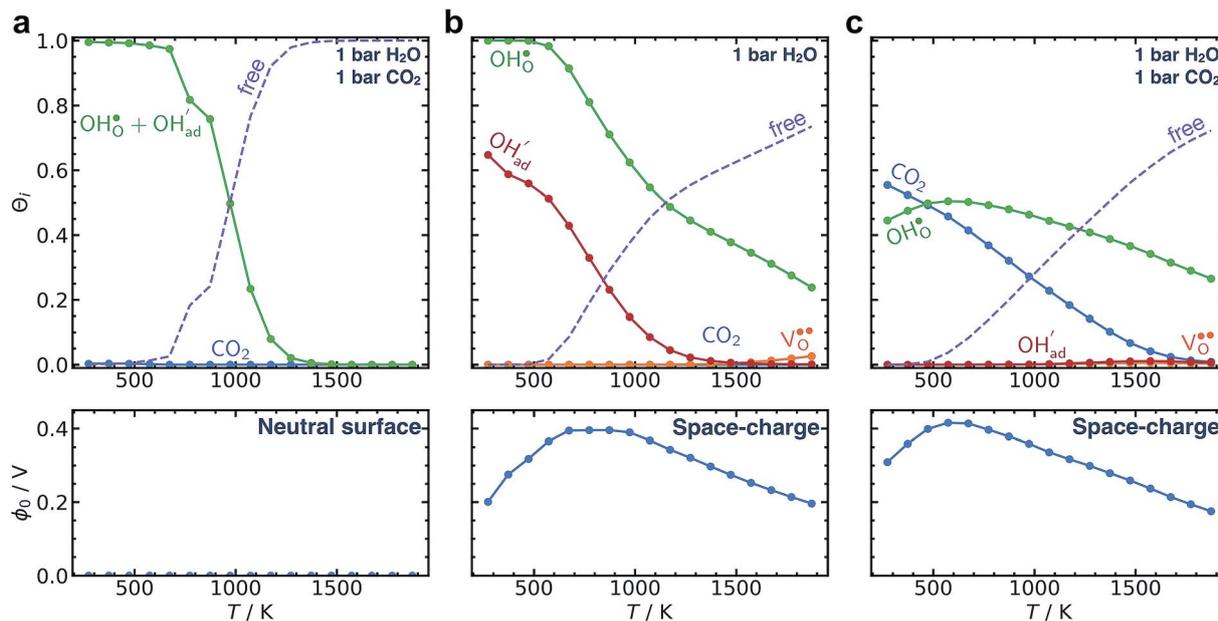


Fig. 7 Surface coverages of adsorbates and defects (protons, oxygen vacancies, hydroxide and carbonate species) as well as free surface sites and space-charge potential as function of temperature calculated without space-charge (a) and without competitive  $\text{CO}_2$  adsorption (b) compared to the complete surface equilibria for  $\text{BaZr}_{0.8}\text{Y}_{0.2}\text{O}_3$  (0 0 1) (c).

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

