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CORRECTION

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Correction: Interplay between H$_2$O and CO$_2$ coadsorption and space-charge on Y-doped BaZrO$_3$ surfaces

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Correction for 'Interplay between H$_2$O and CO$_2$ coadsorption and space-charge on Y-doped BaZrO$_3$ surfaces' by Jonathan M. Polfus *et al.*, *J. Mater. Chem. A*, 2018, **6**, 24823–24830.

The calculated entropies of H$_2$O and CO$_2$ chemisorption presented in Table 2 in the published article, -6.37×10^{-4} eV K^{-1} and -8.78×10^{-4} eV K^{-1}, respectively, were not correct due to an error in the reference value used for gaseous H$_2$O and CO$_2$. The correct adsorption entropies are -1.39×10^{-3} eV K^{-1} for H$_2$O and -1.68×10^{-3} eV K^{-1} for CO$_2$, 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.
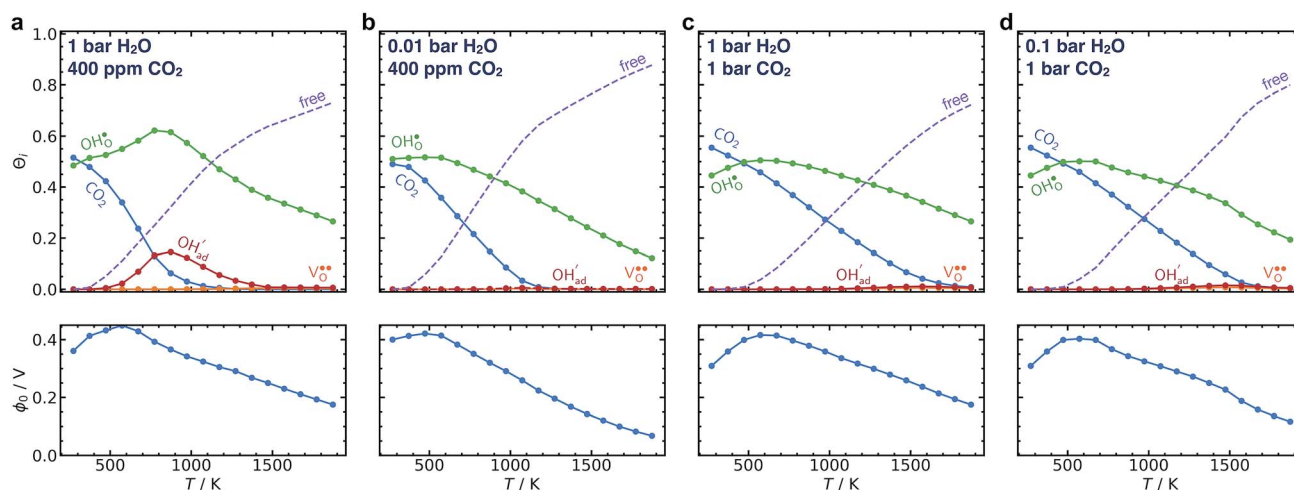

Fig. 4 Surface coverages of adsorbates and defects (protons, oxygen vacancies, hydroxide and carbonate species) as well as free surface sites (top) and the corresponding space-charge potential (bottom) on BaZr$_{0.8}$Y$_{0.2}$O$_3$ (0 0 1) as function of temperature under 1 bar H$_2$O, 400 ppm CO$_2$ (a), 0.01 bar H$_2$O, 400 ppm CO$_2$ (b) and 1 bar CO$_2$, 1 bar H$_2$O (c) and 0.1 bar H$_2$O, 1 bar CO$_2$.

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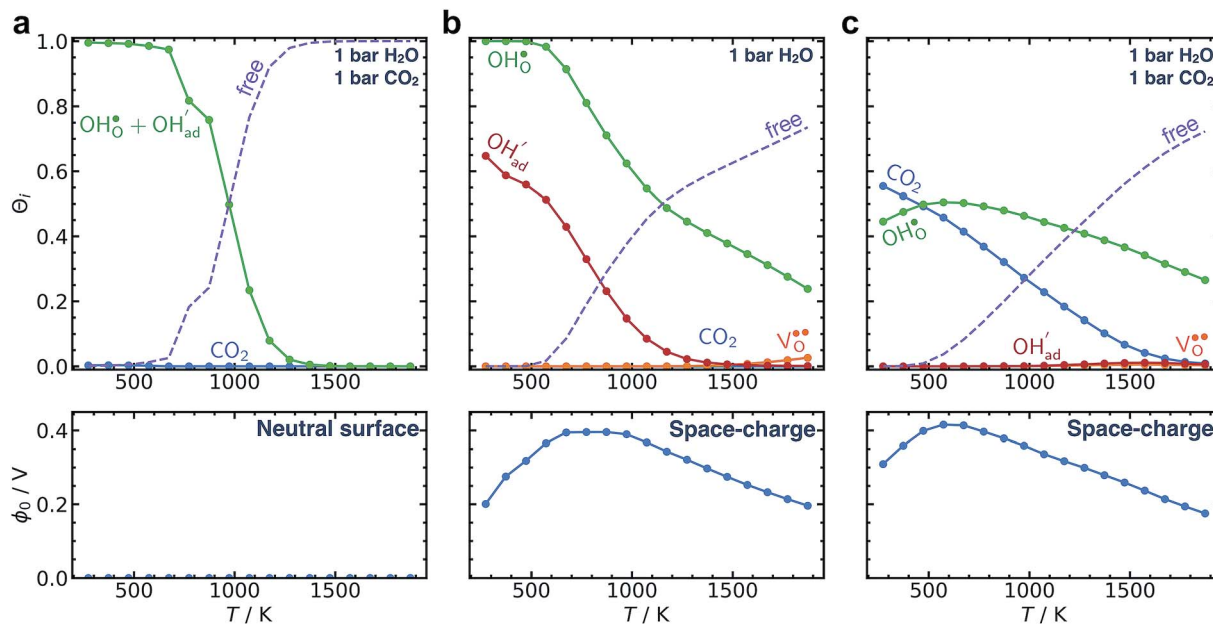
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Fig. 7 Surface coverages of adsorbates and defects (protons, oxygen vacancies, hydroxide and carbonate species) as well as free surface sites and space-charge potential as function of temperature calculated without space-charge (a) and without competitive CO_2 adsorption (b) compared to the complete surface equilibria for $BaZr_{0.8}Y_{0.2}O_3$ (0 0 1) (c).

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