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Correction: Interplay between H₂O and CO₂ coadsorption and space-charge on Y-doped BaZrO₃ surfaces

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Correction for 'Interplay between H₂O and CO₂ coadsorption and space-charge on Y-doped BaZrO₃ surfaces' by Jonathan M. Polfus *et al.*, *J. Mater. Chem. A*, 2018, 6, 24823–24830.

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The calculated entropies of H₂O and CO₂ 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 H₂O and CO₂. The correct adsorption entropies are -1.39×10^{-3} eV K⁻¹ for H₂O and -1.68×10^{-3} eV K⁻¹ for CO₂, 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.

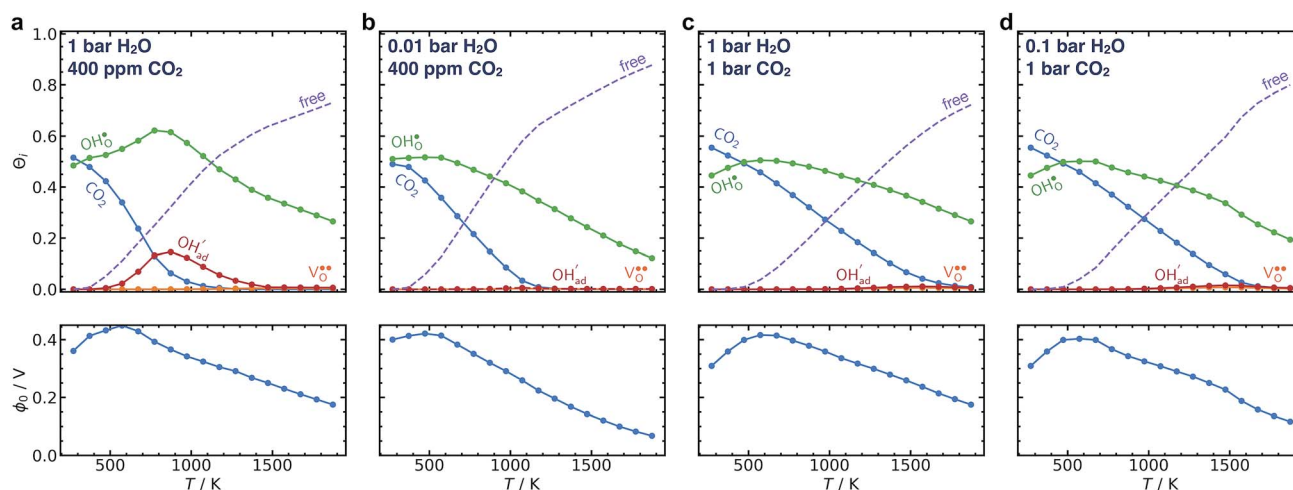


Fig. 4 Surface coverages of adsorbates and defects (protons, oxygen vacancies, hydroxide and carbonate species) as well as free surface sites (top) and the corresponding space-charge potential (bottom) on BaZr_{0.8}Y_{0.2}O₃ (0 0 1) as a function of temperature under 1 bar H₂O, 400 ppm CO₂ (a), 0.01 bar H₂O, 400 ppm CO₂ (b) and 1 bar CO₂, 1 bar H₂O (c) and 0.1 bar H₂O, 1 bar CO₂.

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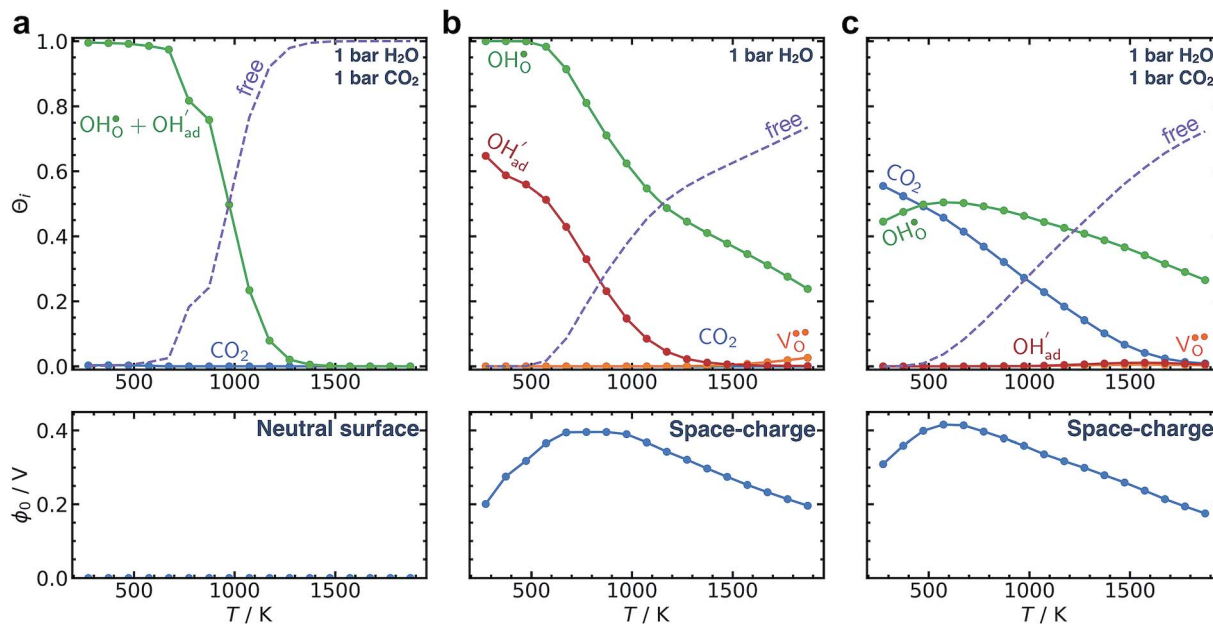


Fig. 7 Surface coverages of adsorbates and defects (protons, oxygen vacancies, hydroxide and carbonate species) as well as free surface sites and space-charge potential as function of temperature calculated without space-charge (a) and without competitive CO_2 adsorption (b) compared to the complete surface equilibria for $\text{BaZr}_{0.8}\text{Y}_{0.2}\text{O}_3$ (0 0 1) (c).

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

