Correction to: Simulated Temperature Programmed Desorption of Acetaldehyde on CeO₂(111): Evidence for the Role of Oxygen Vacancy and Hydrogen Transfer

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The original version of this article unfortunately contained an error in Fig. 6. The authors would like to correct the error with this erratum. The error was due to the missing of a factor of 2 in the rate expression for the surface coverage of atomic H when it desorbs as H₂, and to incorrect settings for some of the initial coverages, in the microkinetic model. A corrected version is shown here as Fig. 6, with the same caption as before.

As a result, the peak desorption temperatures (T_p) of the various species have changed slightly as follows:

Table C1 Changes in peak desorption temperatures of various species

Species	Original T_p (K)	Corrected T_p (K)
Acetaldehyde (AcH)	603	605, with shoulder at ~650
C ₂ H ₄	593	590
C ₂ H ₂	647	654
H ₂	631	613, 671

The corrections bring the outcome of our microkinetic model into better agreement with prior experiments [20, 21], in the following aspects:

- In the simulated TPD the desorption intensity of C₂H₂ is now increased and that of H₂ is reduced, better in line with the TPD results of Chen et al. [20].
- A more pronounced shoulder in the high-temperature desorption of AcH now develops at ~650 K, better in line with the TPD results [20]. Closer inspection of our model suggests that this shoulder is due to the decomposition of the precursor to C₂H₂ (CHCHO/V_o), which supplies an additional amount of atomic H that enables more Enl/V_o to desorb as AcH.
- A certain coverage of Enl/V_o now co-exists with the C–O coupled dimer between ca. 100 and 400 K, in better agreement with the RAIRS results of Calaza et al. [21] in that a minority enolate state was identified by those authors when they annealed AcH on CeO_{2x}(111) to 300 K.

The original article can be found online at <https://doi.org/10.1007/s11244-016-0703-y>.

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Fig. 6 Simulated **a** TPD spectra and **b** corresponding coverages of surface intermediates as a function of temperature for AcH adsorbed on $\text{CeO}_{2-x}(111)$. Initial conditions: total AcH coverage = 0.9 ML; coverages of all other adsorbates = 0 ML; oxygen vacancy coverage = 0.3 ML; temperature = 50 K. Ramp rate = 2 K/s