

CORRECTION

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rsc.li/catalysisCorrection for 'The first-principles-based microkinetic simulation of the dry reforming of methane over Ru(0001)' by Wan-Ying Wang *et al.*, *Catal. Sci. Technol.*, 2021, 11, 1395–1406, DOI: 10.1039/d0cy01942a

The Royal Society of Chemistry regrets an error caused during production, where, in the abstract of the PDF version of the original article a sentence is incomplete. The HTML version of the abstract is correct.

The full and correct abstract is as shown below: The CO₂ reforming of methane (dry reforming) is a challenging reaction because it requires high temperature and is always accompanied by various side reactions, such as steam reforming, the reverse water gas shift reaction, and coke formation. In this study, density functional theory was used to study dry reforming and its related processes on the Ru(0001) surface. The results showed that CO₂ dissociation occurred mainly by direct dissociation and O* produced by CO₂ dissociation was the main oxidant of CH_x* intermediates on the surface of Ru(0001). The activation energy of CO₂ was lower than that of CH₄, and CH–O oxidation and C–O oxidation were likely. The free energy spans of dry reforming, steam reforming, the reverse water gas shift, CH₄ cracking, and the Boudouard reaction were 158, 155, 123, 176, and 245 kJ mol^{−1}, respectively. We compared the same key process on the surfaces of Ni(111) and Ru(0001), and the results showed that Ru was more resistant to coke than Ni due to its strong “oxophilic” nature, which resulted in a facile activation of CO₂. Interestingly, it was found that the binding energy difference between CH_x* and O* increased following the order Ru > Co > Ni > Pd > Pt, and the same trend for the carbon deposition resistance could be expected. The results of the microkinetic simulation under catalytic reaction conditions (973.15 K, 1 bar) and low-pressure conditions (973.15 K, 160 Pa) showed that the ratio of the generation rate of H₂ and CO was slightly less than 1 : 1 and a small amount of H₂O was generated, which indicates that the reverse water gas shift reaction and steam reforming had little effect on the dry reforming. The activation of CH₄ was the rate-limiting step in dry reforming, which was confirmed in the sensitivity analysis under catalytic reaction conditions. The dry reforming rate positively correlated with the CH₄ pressure and was almost independent of the CO₂ pressure under low-pressure conditions. In addition, the effect of carbon deposition on the catalyst was very small throughout the simulation process. Our present results may provide a theoretical guide for the experiment and design of a highly efficient dry reforming catalyst by alloying a typical DRM catalyst, such as Ni, with smaller noble Ru to promote its carbon deposition resistance.

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

