A combined EXAFS, XRD, DRIFTS and DFT study of nano copper-based catalysts for CO_2 hydrogenation

Supplementary Material

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1. Continuous hydrothermal flow synthesis

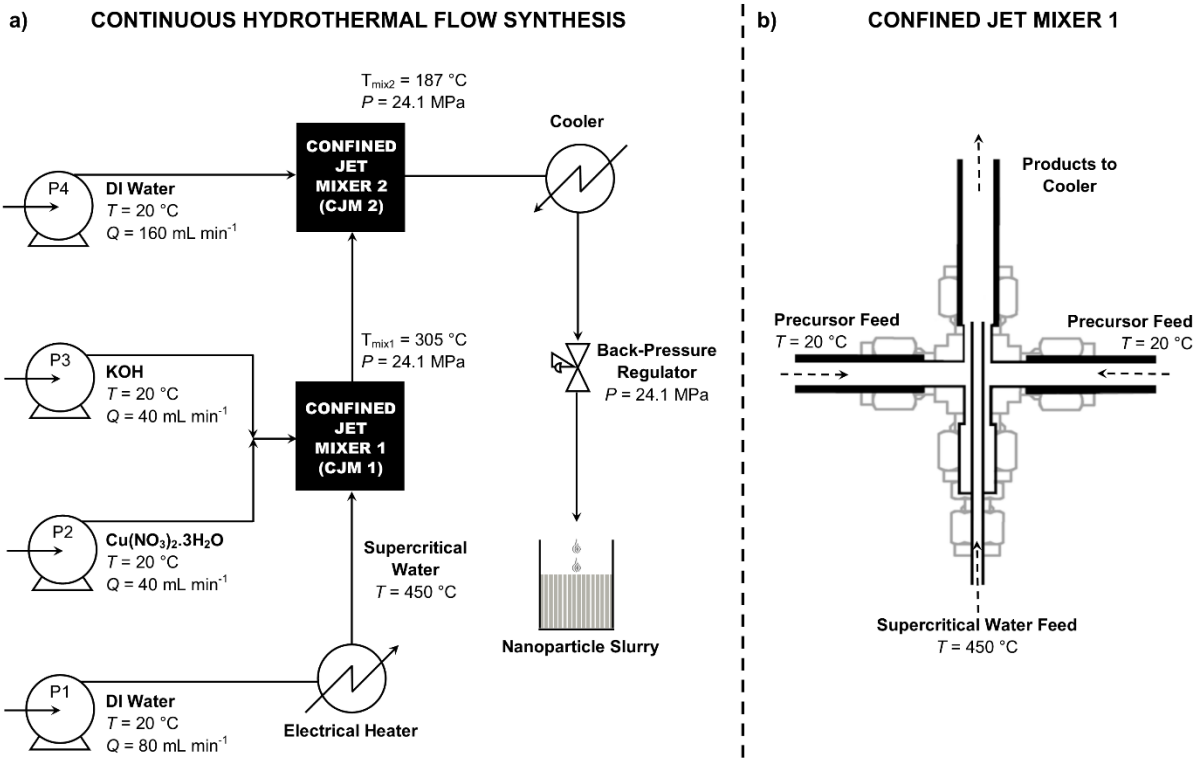

Figure S1 – Schematic representation of the Continuous Hydrothermal Flow Synthesis (CHFS) process using supercritical water for the synthesis of ultrafine copper oxide nanoparticles in flow. Pumps are denoted by P, confined jet mixers are denoted as CJM1 and CJM2.

2. DFT

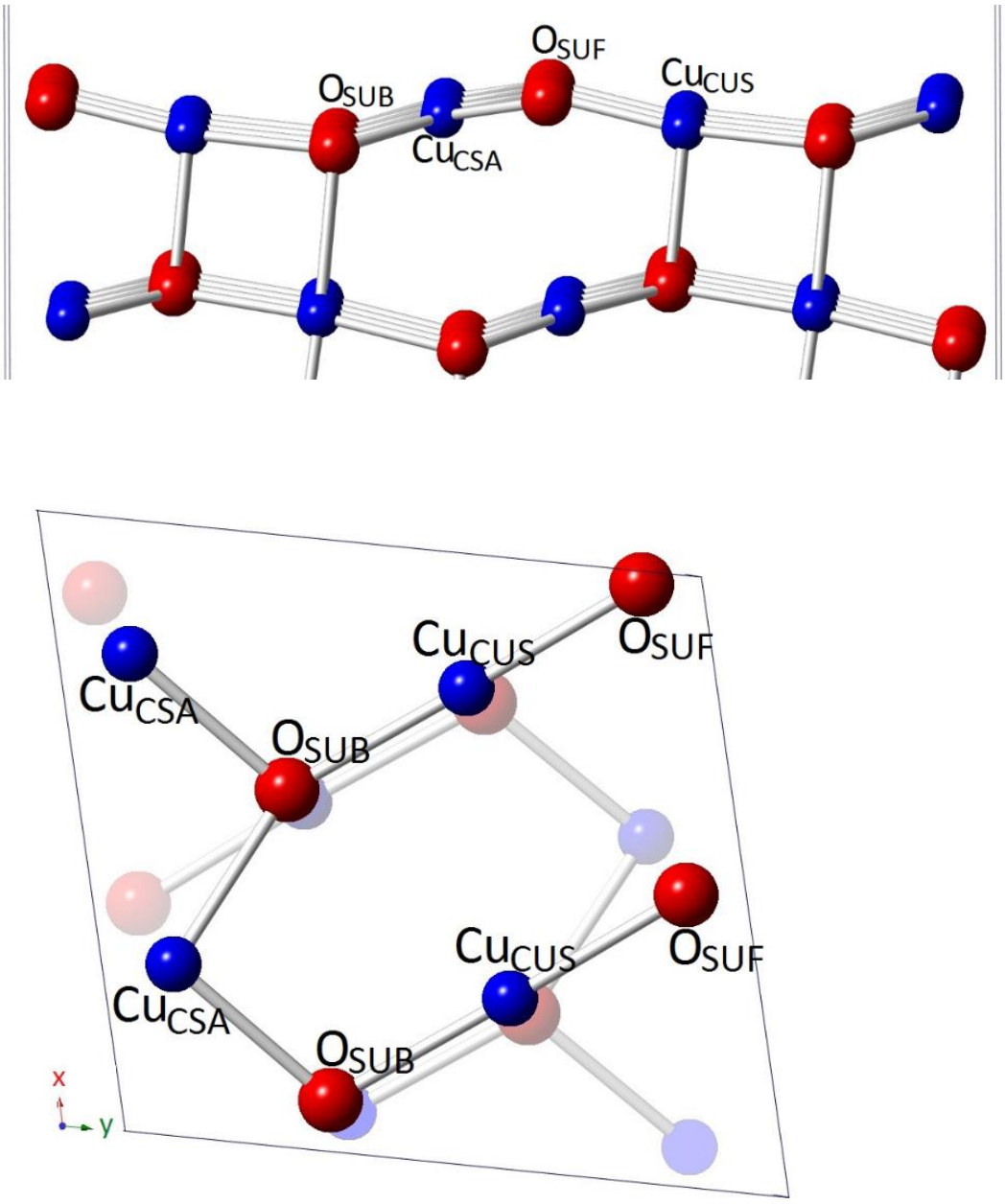

Fig. S2. Side (upper panel) and top (lower panel) views of the CuO(111) surface.

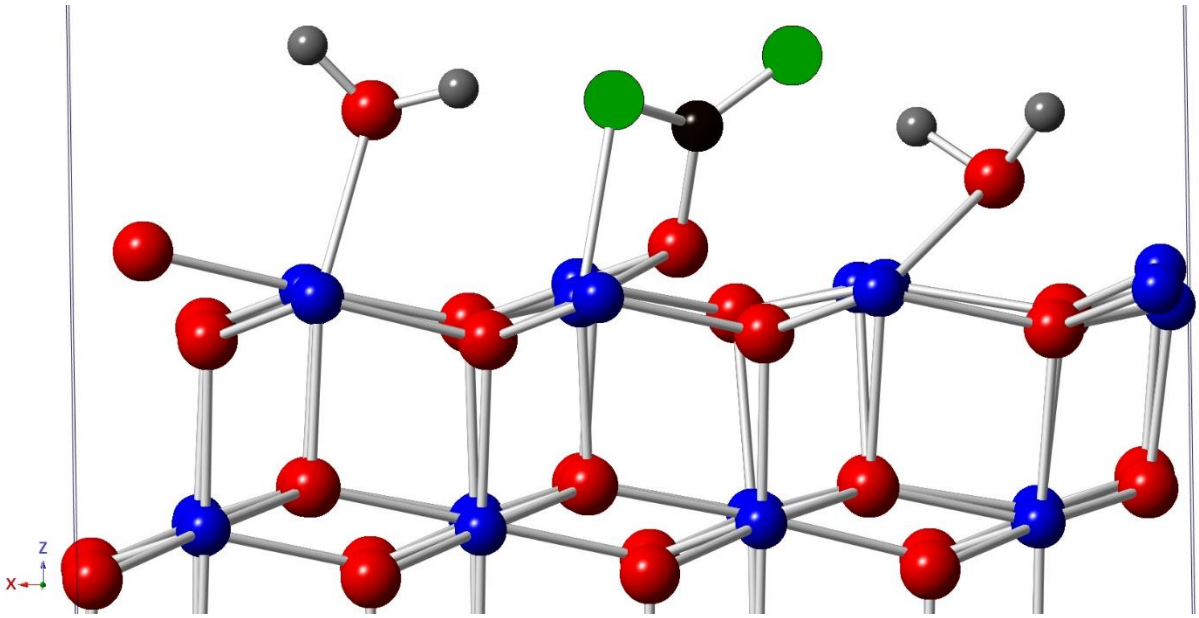

Fig. S3. The co-adsorption of one CO_2 and two H_2 molecules on the CuO(111) surface. Bond length values are in Å. Blue and red colour balls indicate Cu and O surface atoms respectively, while O, C and H atoms of the molecule are represented by green, black and grey colour balls respectively.

3. Heterogeneous tests

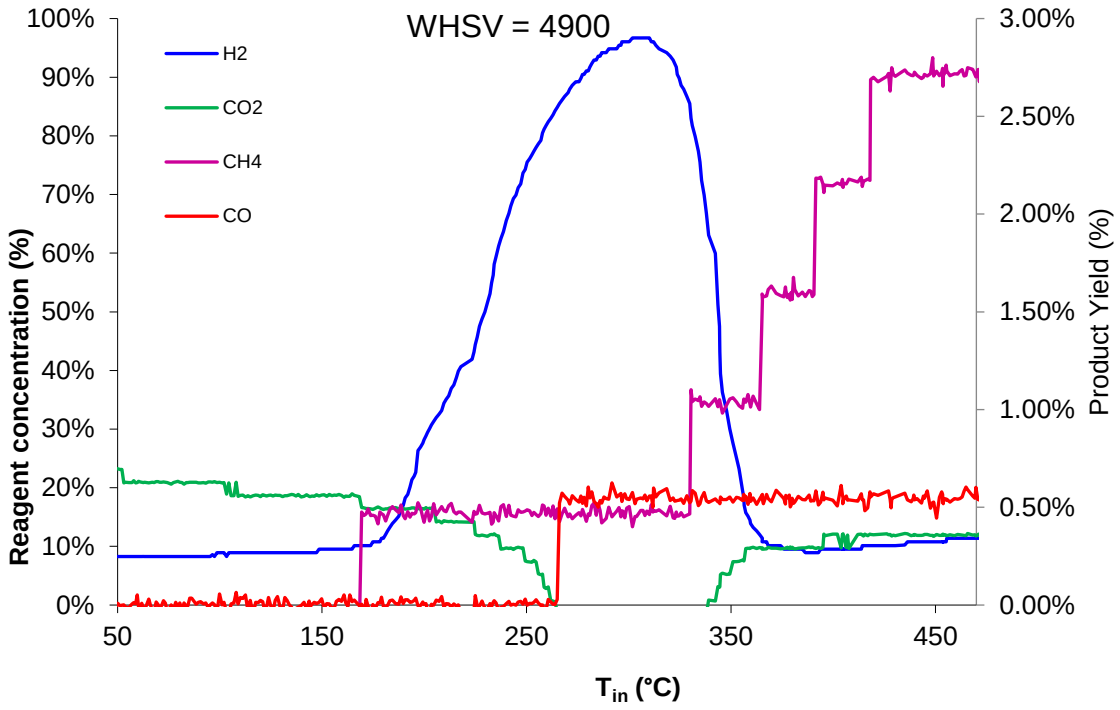

Fig. S4. CO_2 hydrogenation, heterogeneous catalysis tests for CuO-based nanocatalysts. Reagent concentration and product conversion yield vs temperature (50 -500 °C, WHSV = 4900 mL h^{-1} g^{-1}).

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Author Contributions

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