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A combined EXAFS, XRD, DRIFTS and DFT study of nano copper-based catalysts for CO₂ hydrogenation

Supplementary Material

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1. Continuous hydrothermal flow synthesis

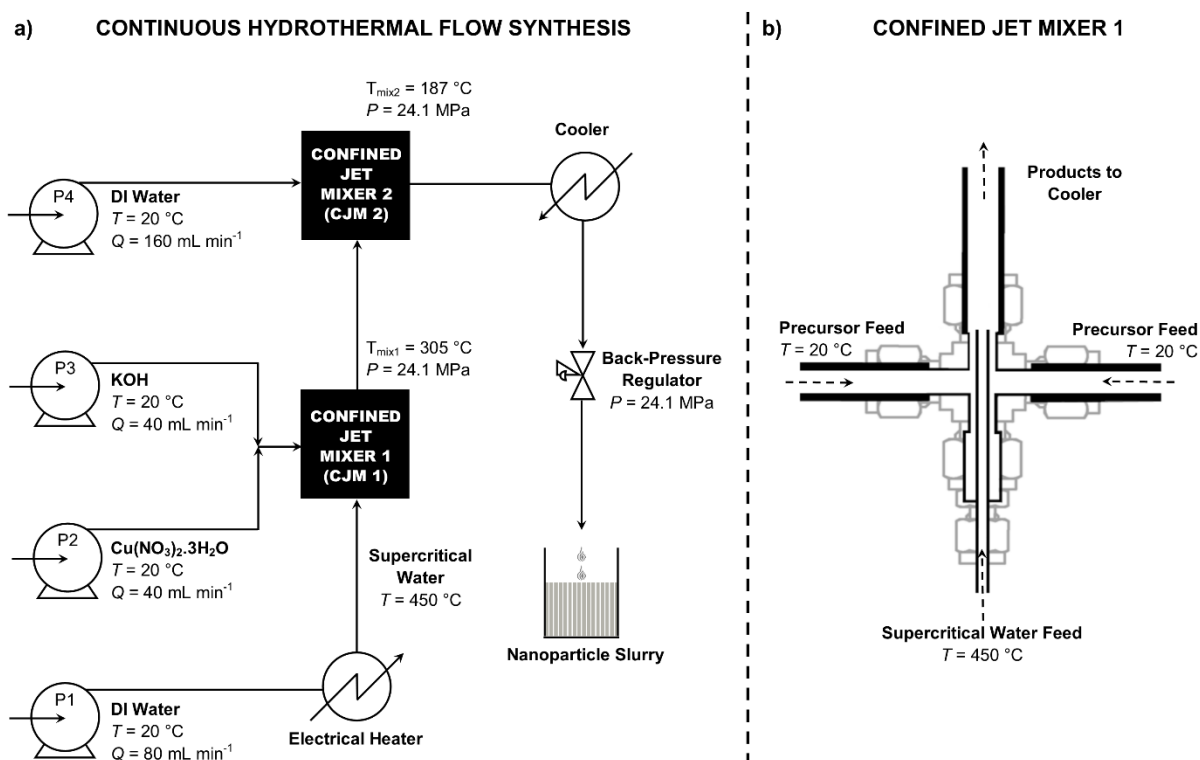


Figure S1 – Schematic representation of the Continuous Hydrothermal Flow Synthesis (CHFS) process using supercritical water for the synthesis of ultrafine copper oxide nanoparticles in flow. Pumps are denoted by P, confined jet mixers are denoted as CJM1 and CJM2.

2. DFT

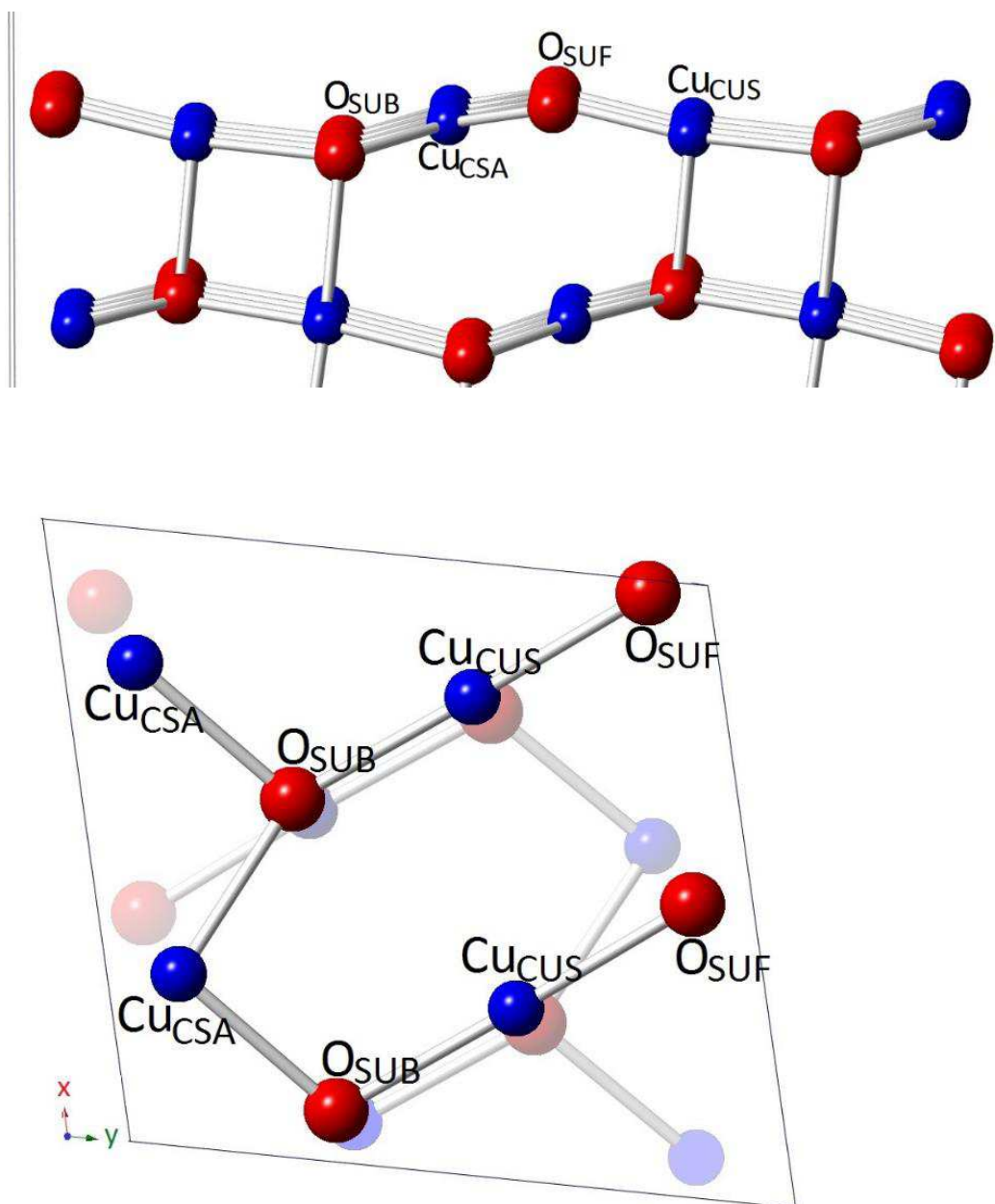


Fig. S2. Side (upper panel) and top (lower panel) views of the CuO(111) surface.

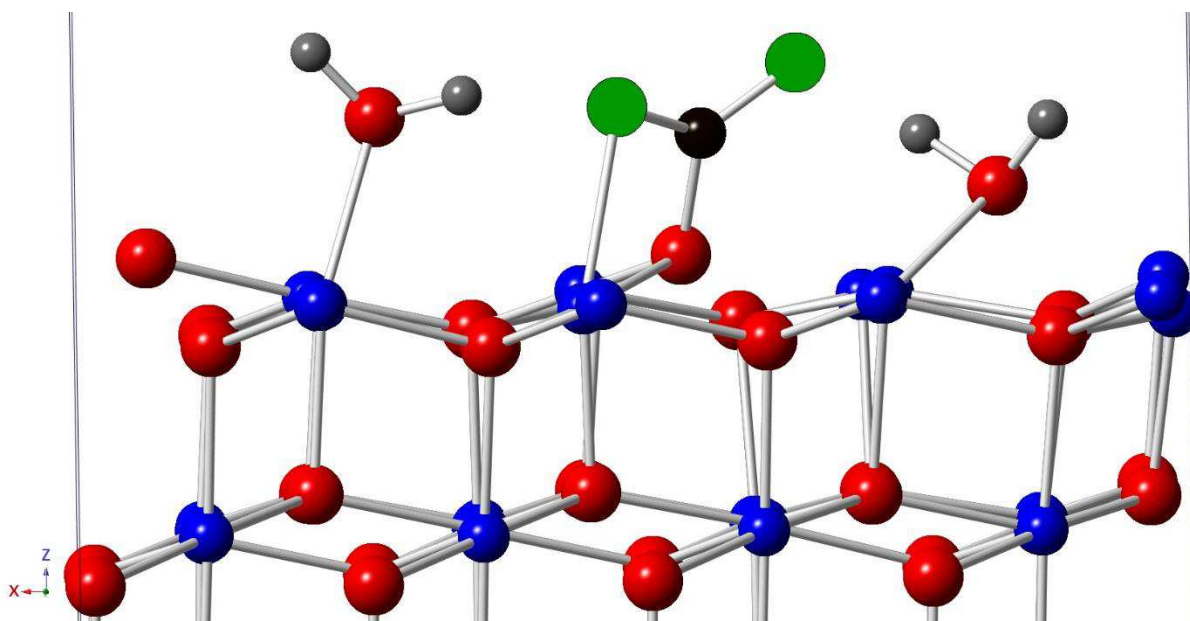


Fig. S3. The co-adsorption of one CO₂ and two H₂ molecules on the CuO(111) surface. Bond length values are in Å. Blue and red colour balls indicate Cu and O surface atoms respectively, while O, C and H atoms of the molecule are represented by green, black and grey colour balls respectively.

3. Heterogeneous tests

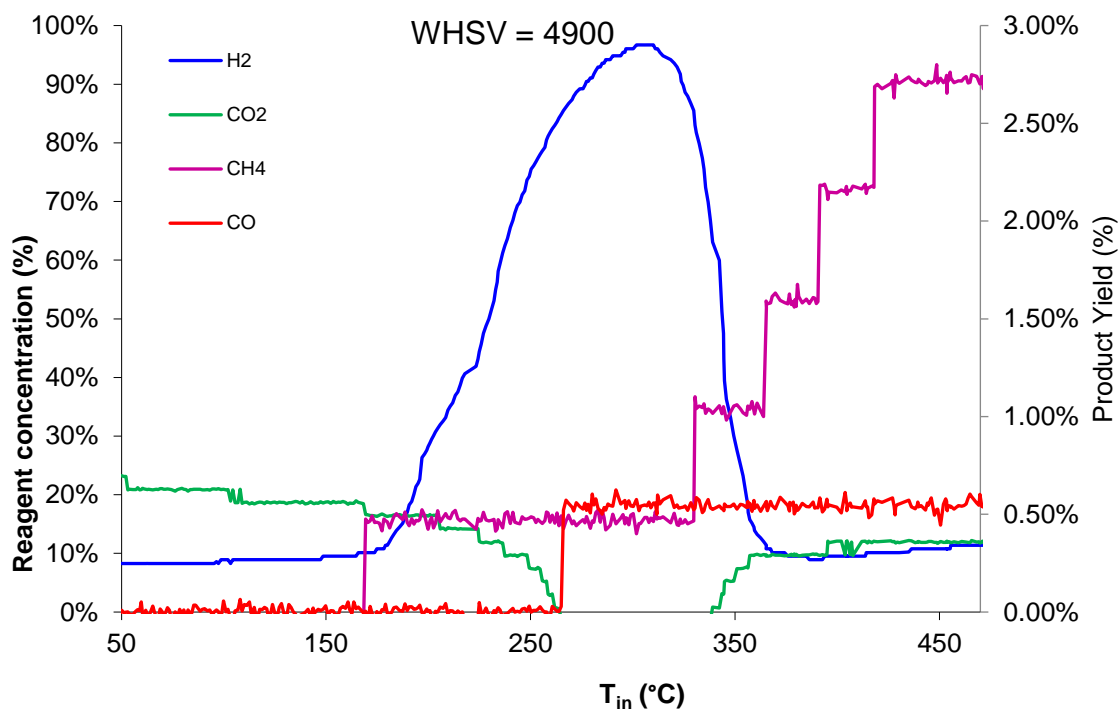


Fig. S4. CO₂ hydrogenation, heterogeneous catalysis tests for CuO-based nanocatalysts. Reagent concentration and product conversion yield vs temperature (50 -500 °C, WHSV = 4900 mL h⁻¹ g⁻¹).

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Author Contributions

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