

This is an Open Access document downloaded from ORCA, Cardiff University's institutional repository: <https://orca.cardiff.ac.uk/id/eprint/95276/>

This is the author's version of a work that was submitted to / accepted for publication.

Citation for final published version:

Bersani, Marco, Gupta, Kalyani, Mishra, Abhishek Kumar, Lanza, Roberto, Taylor, S. F. Rebecca, Islam, Husn-Ubayda, Hollingsworth, Nathan, Hardacre, Christopher, De Leeuw, Nora H. and Darr, Jawwad A. 2016. Combined EXAFS, XRD, DRIFTS, and DFT study of nano copper-based catalysts for CO₂ Hydrogenation. *ACS Catalysis* 6 (9) , pp. 5823-5833. 10.1021/acscatal.6b01529

Publishers page: <http://dx.doi.org/10.1021/acscatal.6b01529>

Please note:

Changes made as a result of publishing processes such as copy-editing, formatting and page numbers may not be reflected in this version. For the definitive version of this publication, please refer to the published source. You are advised to consult the publisher's version if you wish to cite this paper.

This version is being made available in accordance with publisher policies. See <http://orca.cf.ac.uk/policies.html> for usage policies. Copyright and moral rights for publications made available in ORCA are retained by the copyright holders.



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

Supplementary Material

*Marco Bersani^{‡,1}, Kalyani Gupta^{‡,1}, Abhishek Kumar Mishra¹, Roberto Lanza², S.F. Rebecca Taylor³, Husn-Ubayda Islam⁴, Nathan H. Hollingsworth¹, Christopher Hardacre³, Nora H. de Leeuw^{1,4}, Jawwad A. Darr^{*1}*

¹Department of Chemistry, Christopher Ingold Laboratories, University College London, 20 Gordon Street, London, WC1H 0AJ, United Kingdom

²Department of Chemical Engineering and Technology, KTH – Royal Institute of Technology, Teknikringen 42, 100 44 Stockholm, Sweden

³School of Chemical Engineering and Analytical Science, The University of Manchester, Oxford Road, Manchester, M13 9PL, UK

⁴School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, UK

1. Continuous hydrothermal flow synthesis

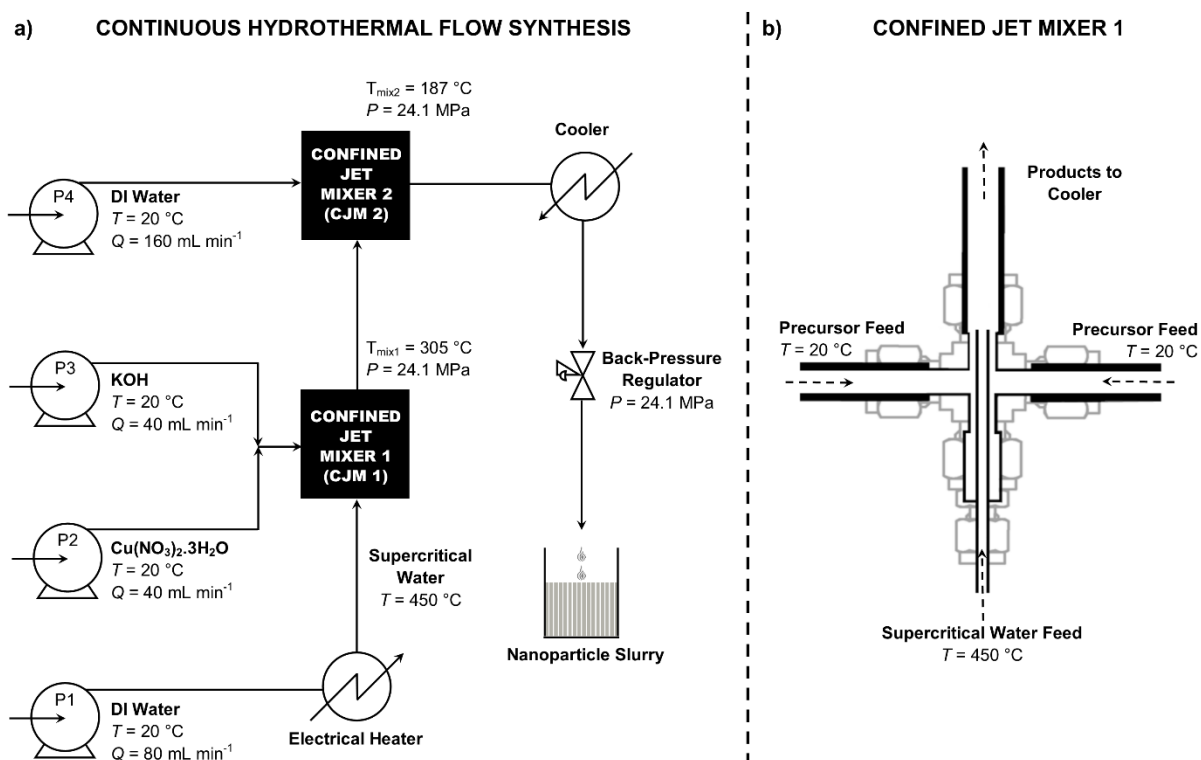


Figure S1 – Schematic representation of the Continuous Hydrothermal Flow Synthesis (CHFS) process using supercritical water for the synthesis of ultrafine copper oxide nanoparticles in flow. Pumps are denoted by P, confined jet mixers are denoted as CJM1 and CJM2.

2. DFT

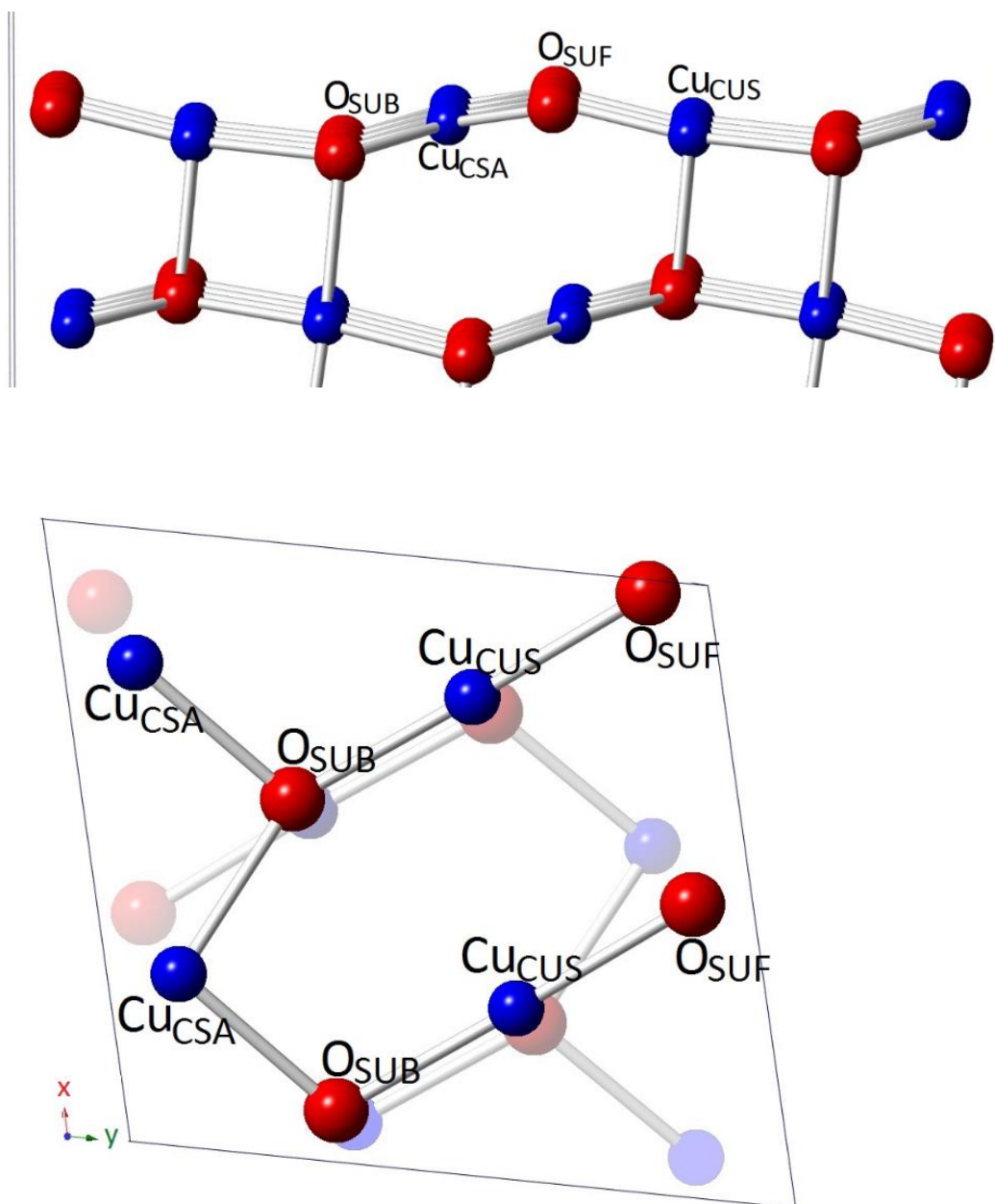


Fig. S2. Side (upper panel) and top (lower panel) views of the CuO(111) surface.

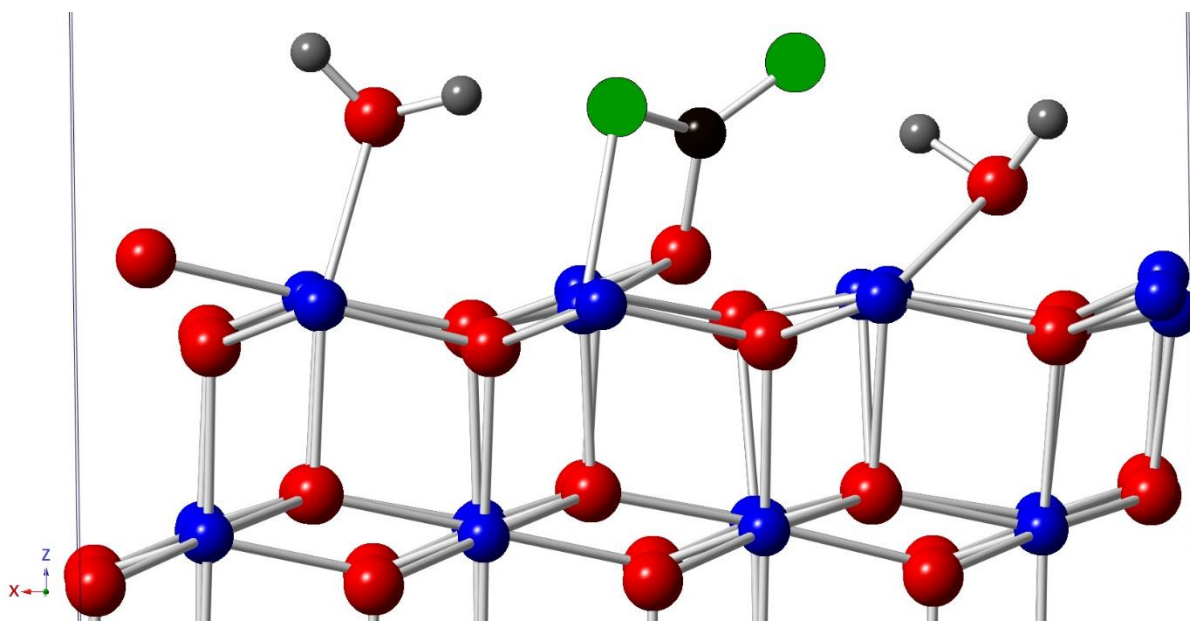


Fig. S3. The co-adsorption of one CO₂ and two H₂ molecules on the CuO(111) surface. Bond length values are in Å. Blue and red colour balls indicate Cu and O surface atoms respectively, while O, C and H atoms of the molecule are represented by green, black and grey colour balls respectively.

3. Heterogeneous tests

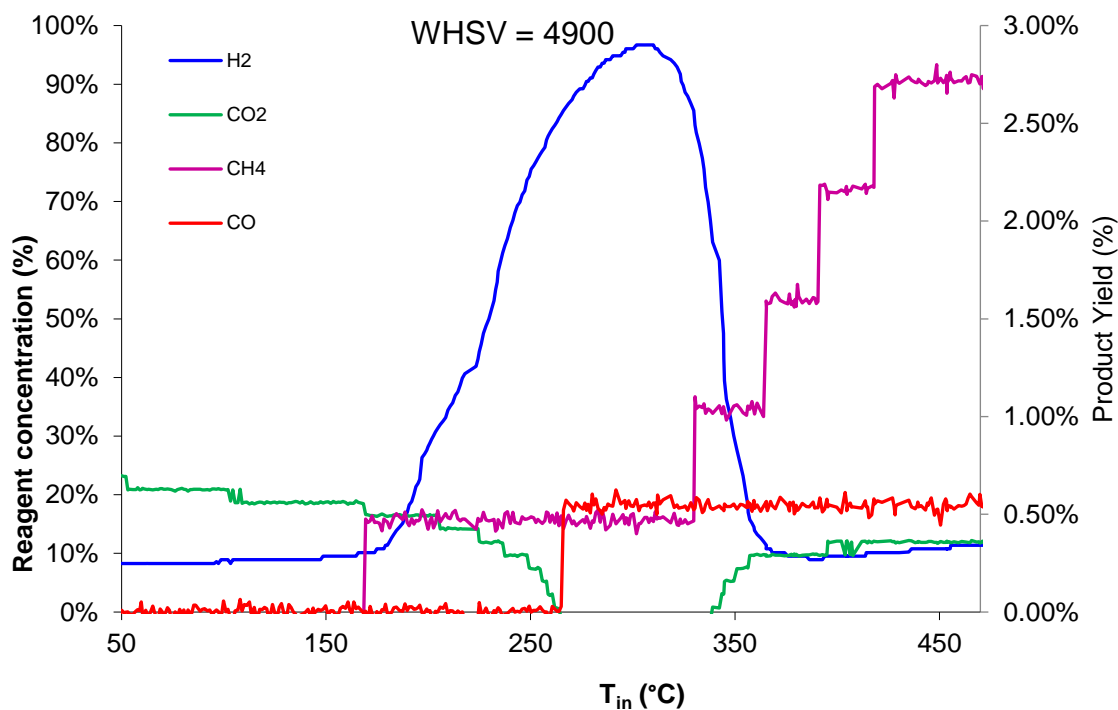


Fig. S4. CO₂ hydrogenation, heterogeneous catalysis tests for CuO-based nanocatalysts. Reagent concentration and product conversion yield vs temperature (50 -500 °C, WHSV = 4900 mL h⁻¹ g⁻¹).

AUTHOR INFORMATION

Corresponding Author

*E-mail: j.a.darr@ucl.ac.uk. Telephone: +44 (0)20 7679 4345

Author Contributions

‡These authors contributed equally.