

SUPPORTING INFORMATION

Carbon Capture by Metal Oxides: Unleashing the Potential of the (111) Facet

Greg A. Mutch,^{*,†,‡} Sarah Shulda,[§] Alan J. McCue,[‡] Martin J. Menart,[§] Cristian V. Ciobanu,^{||} Chilan Ngo,[§] James A. Anderson,[‡] Ryan M. Richards[§] and David Vega-Maza[‡]

[†]School of Engineering, Newcastle University, Newcastle upon Tyne NE1 7RU, United Kingdom.

[‡]School of Engineering, University of Aberdeen, Aberdeen AB24 3FX, United Kingdom.

[§]Department of Chemistry and Geochemistry, Colorado School of Mines, Golden, Colorado 80401, United States.

^{||}Department of Mechanical Engineering and Materials Science Program, Colorado School of Mines, Golden, Colorado 80401, United States.

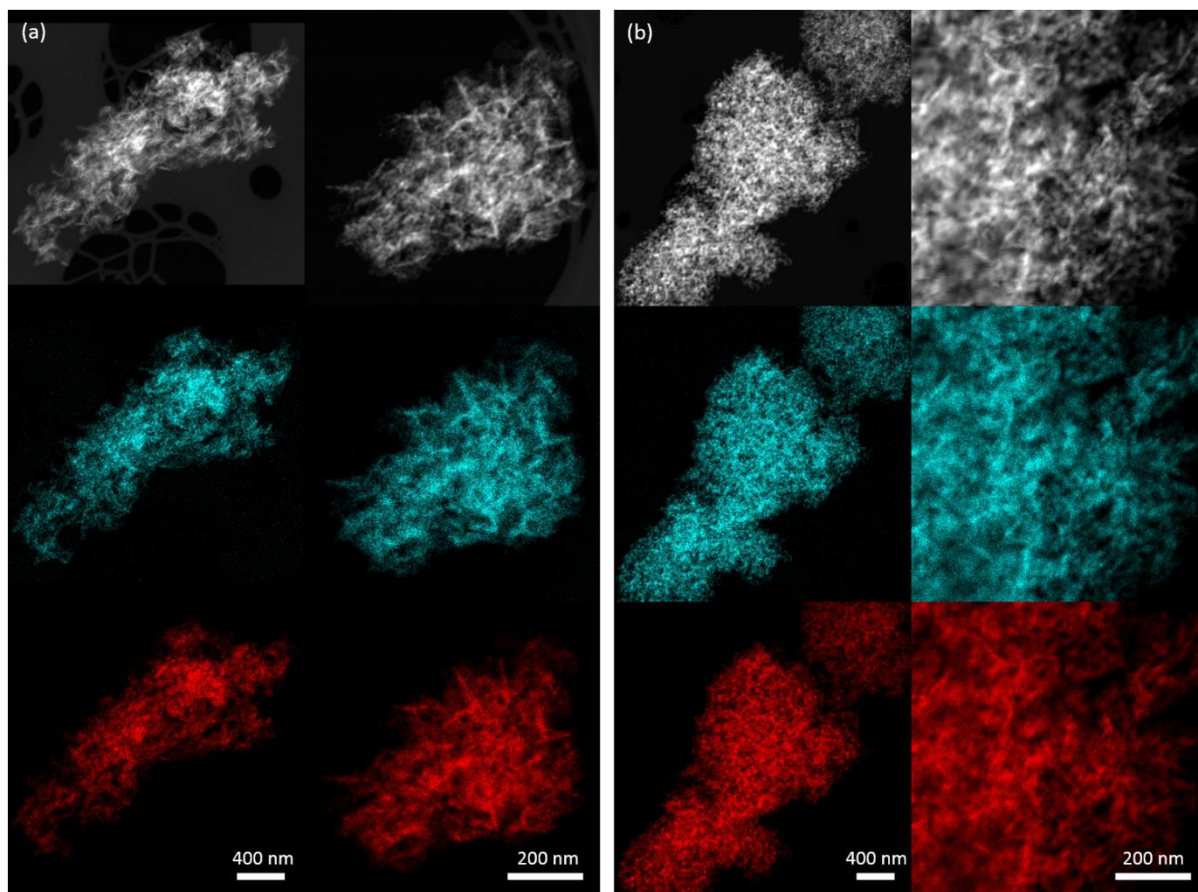


Figure S1. Scanning transmission electron microscopy (STEM) and energy dispersive X-ray spectroscopy (EDS) for (a) MgO(111) and (b) MgO(111) 800°C. Morphology and compositional homogeneity remain consistent after heat treatment. (STEM = White, O = Blue, Mg = Red).

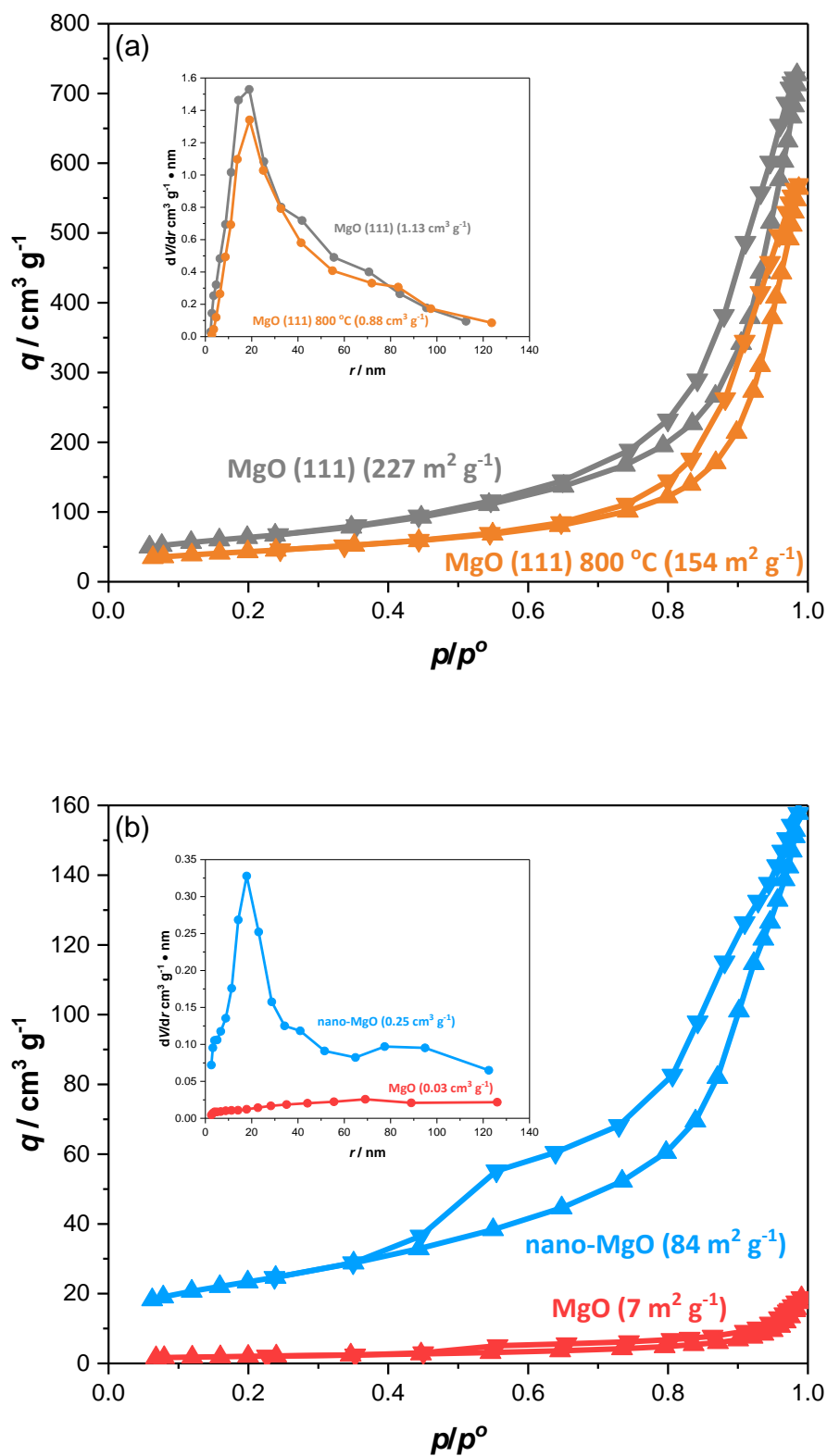


Figure S2. Nitrogen adsorption-desorption isotherms and pore size distributions (inset) for (a) MgO(111) and MgO(111) 800°C and (b) nano-MgO and MgO. Specific surface area values, as determined by the BET method are inset as well as pore volumes as determined by the BJH method.

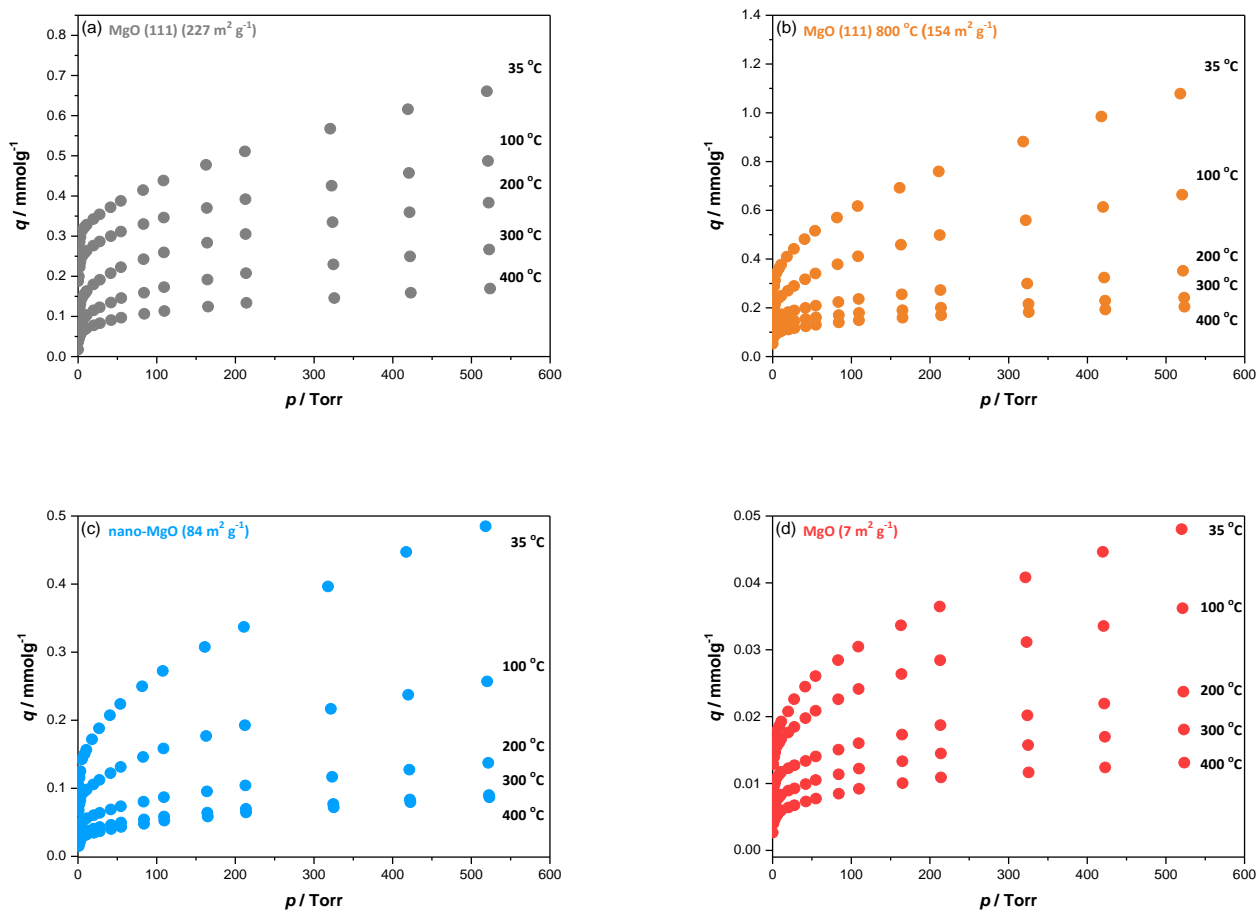


Figure S3. CO₂ adsorption isotherms for (a) MgO(111), (b) MgO(111) 800°C, (c) nano-MgO and (d) MgO with specific surface areas inset. T_{ads} = 35, 100, 200, 300 and 400°C and p_{CO_2} = 0.05 – 520 Torr.

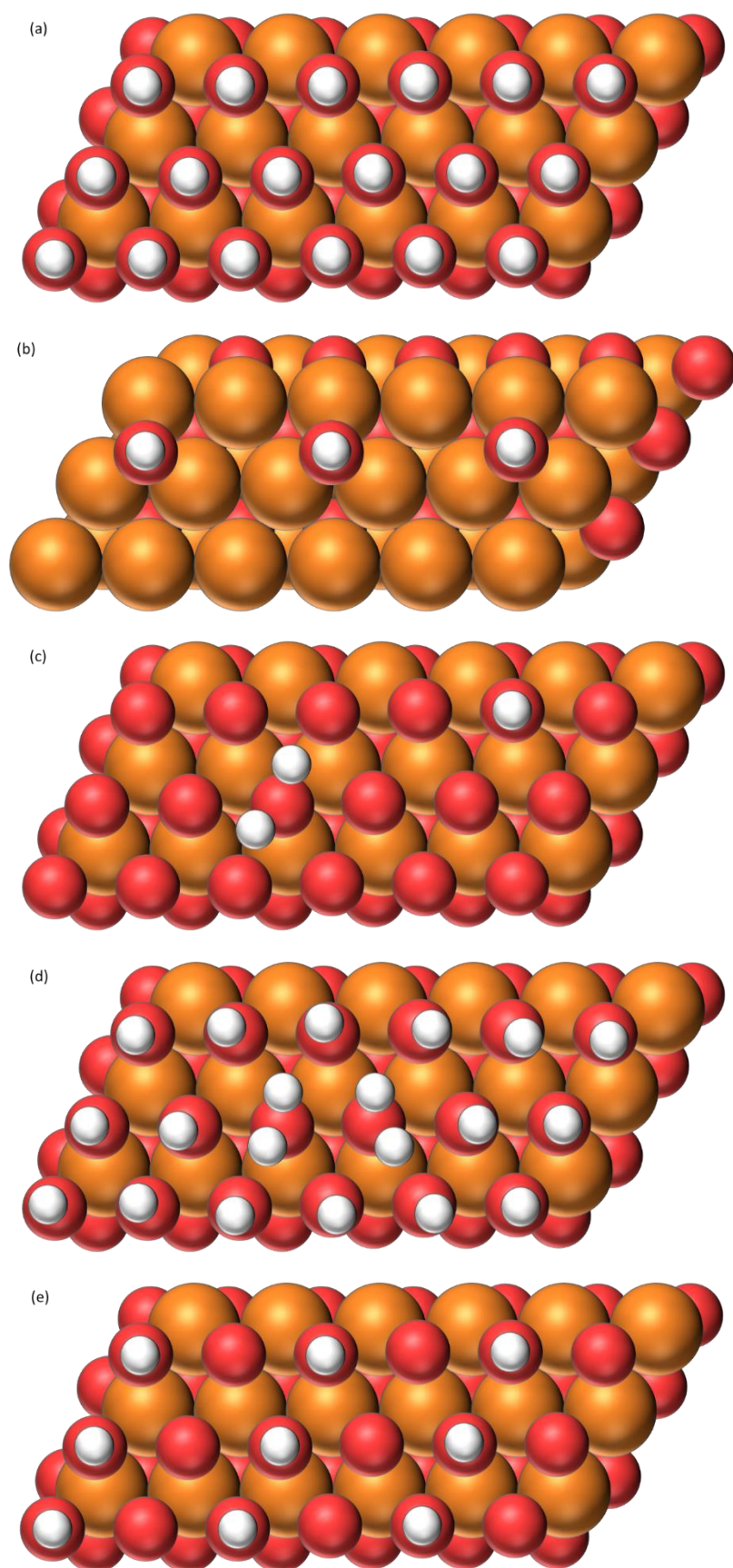


Figure S4. Top view configurations of hydroxyl and water on a 6x3 MgO(111) surface cell for DFT calculations. (a) 100% H-covered O-terminated surface, (b) low coverage of OH Mg-terminated surface, (c) one water and one OH O-terminated surface, (d) two waters on otherwise H-covered O-terminated surface and (e) 50% H-covered O-terminated surface. (Mg = Orange, O = Red and H = White).

Table S1. Basic site quantification for MgO(111) and MgO(111) 800°C, as determined by CO₂-TPD, with weak ($T_d < 120^\circ\text{C}$), intermediate ($T_d = 120 - 275^\circ\text{C}$) and strong ($T_d > 275^\circ\text{C}$) basic sites, as well as total.

Sample	Basic sites at desorption temperature (T_d) [$\mu\text{mol g}^{-1}$]			Total
	< 120 [$^\circ\text{C}$]	120 – 275 [$^\circ\text{C}$]	> 275 [$^\circ\text{C}$]	
MgO(111)	121	184	52	357
MgO(111) 800°C	122	240	55	415