

Supporting Information

Carbon formation mechanism of C₂H₂ in Ni based catalysts revealed by *in situ* electron microscopy and molecular dynamics simulations

Chunwen Sun^{1,2,6*}, Rui Su^{3,5}, Jian Chen^{4*}, Liang Lu,¹ Pengfei Guan^{3*}

¹CAS Center for Excellence in Nanoscience, Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing 100083, P. R. China

²School of Nanoscience and Technology, University of Chinese Academy of Sciences, Beijing 100049, P. R. China

³Beijing Computational Science Research Center, Beijing 100193 China

⁴Nanotechnology Research Centre, National Research Council Canada (NRC), Edmonton, Alberta T6G 2M9, Canada

⁵Innovative Center for Advanced Materials, Hangzhou Dianzi University, Hangzhou 310018, China

⁶Center on Nanoenergy Research, School of Physical Science and Technology, Guangxi University, Nanning 530004, P.R. China

* Corresponding authors.

E-mail: sunchunwen@binn.cas.cn (C. Sun); jian.chen@nrc-cnrc.gc.ca (J. Chen) and pguan@csrc.ac.cn (P. Guan)

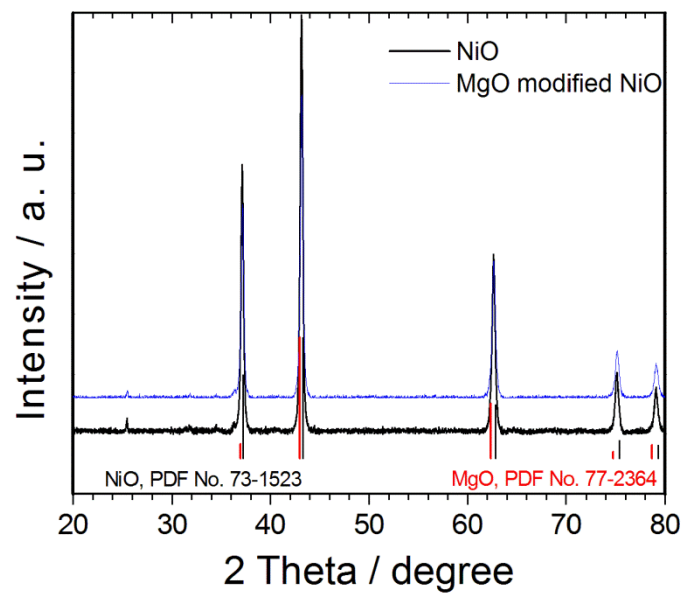


Figure S1. XRD patterns of NiO and MgO modified NiO samples.

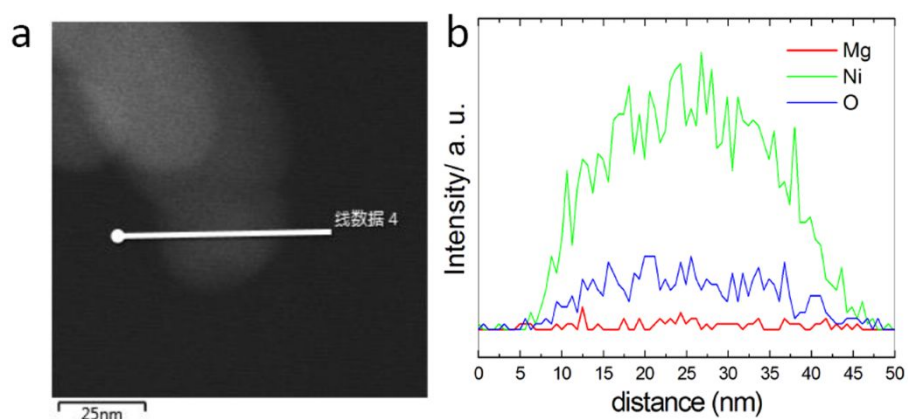
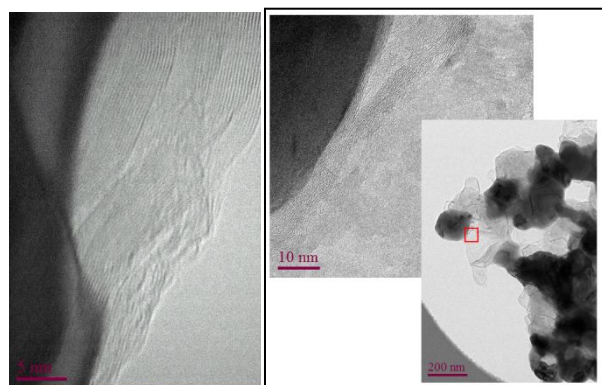


Figure S2. (a) ADF STEM image of MgO modified NiO particle and (b) The line scanning profiles of elements across the particle in (a).



(a)

(b)

Figure S3. (a) TEM image showing graphitic layers formed in NiO sample at 800°C under $\text{H}_2+\text{C}_2\text{H}_2$. Electron energy loss spectrum (EELS) confirms it is carbon. (b) TEM image showing graphitic layers formed in MgO modified NiO sample at 800°C under $\text{H}_2+\text{C}_2\text{H}_2$. The upper left image is the HRTEM of the region marked by the red square in the low magnification image.