Supplementary Materials: Tandem Hydrogenation/Hydrogenolysis of Furfural to 2-Methylfuran over a Fe/Mg/O Catalyst: Structure–Activity Relationship

Carlo Lucarelli, Danilo Bonincontro, Yu Zhang, Lorenzo Grazia, Marc Renom-Carrasco, Chloé Thieuleux, Elsje Alessandra Quadrelli, Nikolaos Dimitratos, Fabrizio Cavani and Stefania Albonetti *

Pyridine Adsorption Desorption IR Analysis

In order to investigate the types of acid sites, the Py-FTIR spectra were recorded. **Figure S1** shows the IR spectra of adsorbed pyridine over FeO_x/MgO_1_10 at different temperatures. The absence of band at 1540 cm⁻¹ that are the characteristic band of Brønsted acid, the band at 1442 cm⁻¹, corresponding to the adsorption of Pyridine at the Lewis acid sites (PyL) indicated that only Lewis acid presence in Fe containing MgO catalysts. In order to evaluate the strengths of the acid sites (Lewis acid sites), the spectrum was collected after evacuation at different temperatures. The weak sites are defined as the ones from which pyridine is removed by evacuation at 200 °C; the medium strength corresponds to evacuation between 200 and 400 °C and the strong sites remain adsorbing pyridine after evacuation at 400 °C. It is evident that the two samples (Fe/Mg/O_1_2 and FeOx/MgO_1_10) just exhibited Lewis acidity and Fe/Mg/O_1_2 had much more medium acidic sites than FeOx/MgO_1_10 samples. Sample Fe/Mg/O_1_10 presented less acidity. The acidity quantify was used pyridine IR spectra and base on the equation based on the literature.



Figure S1. Pyridine-FTIR <u>spectra</u> of Fe/Mg/O_1_1 obtained after evacuation at different temperatures. (a) room temperature; (b) 100 °C; (c) 200 °C; (d) 300 °C and (e) 400 °C.



Figure S2. Pyridine-FTIR <u>spectra</u> of Fe/Mg/O_1_2 obtained after evacuation at different temperatures. (a) room temperature; (b) 100 °C; (c) 200 °C; (d) 300 °C and (e) 400 °C.



Figure S3. Pyridine-FTIR spectra of FeOx/MgO_1_10 obtained after evacuation at different temperatures. (**a**) room temperature (**b**) 100 °C; (**c**) 200 °C; (**d**) 300 °C and (**e**) 400 °C.



Figure S4. Pyridine-FTIR spectra of FeO_x/MgO_1_2 obtained after evacuation at different temperatures. (a) room temperature; (b) 100 °C; (c) 200 °C; (d) 300 °C and (e) 400 °C.



Figure S5. Furfural adsorption and desorption over MgO sample from RT to 400 °C.



Figure S6. Furfural adsorption / desorption over FeOx/MgO_1_10 sample from RT to 400 °C.



Figure S7. FTIR Spectra of Furfuryl alcohol adsorption /desorption Over MgO at different temperature.



Figure S8. Furfuryl alcohol adsorption /desorption over FeO_x/MgO_1_10 within different temperature.