Electronic Supplementary Information (ESI)

The role of speciation of Ni^{2+} and its interaction with support for selectivity and stability in conversion of ethylene to propene

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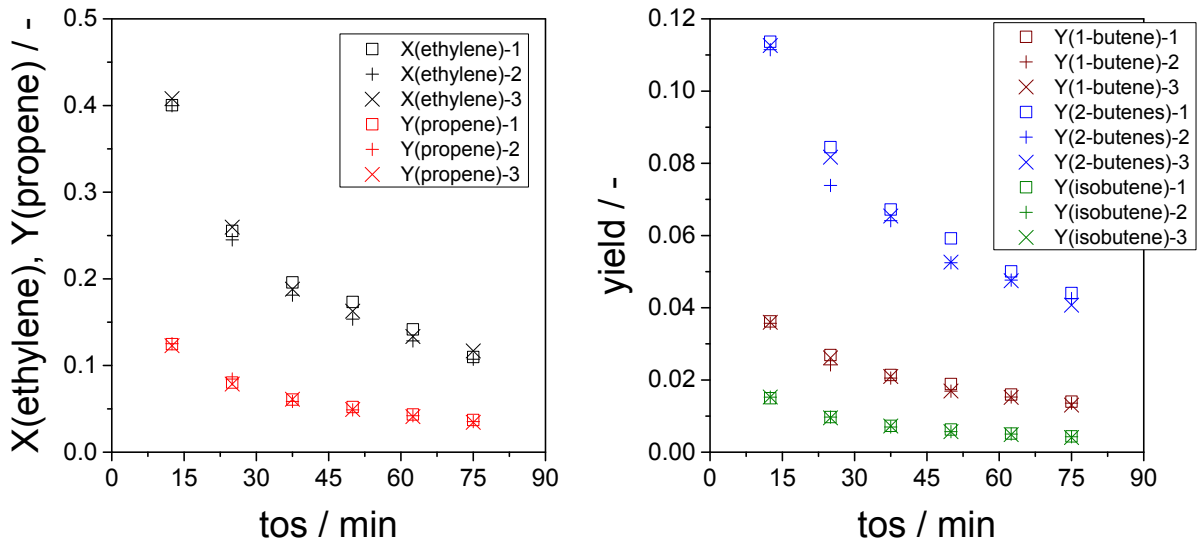

Figure S1 Reproducibility of catalytic tests in three reactors of the 15-fold parallel fixed-bed reactor. Reaction conditions per reactor: 0.25 g of 2Ni/Siral70_gr, gas flow rate 17.5 mL·min^{-1} 10vol% ethylene in N_2, T=375 °C, p=1bar.

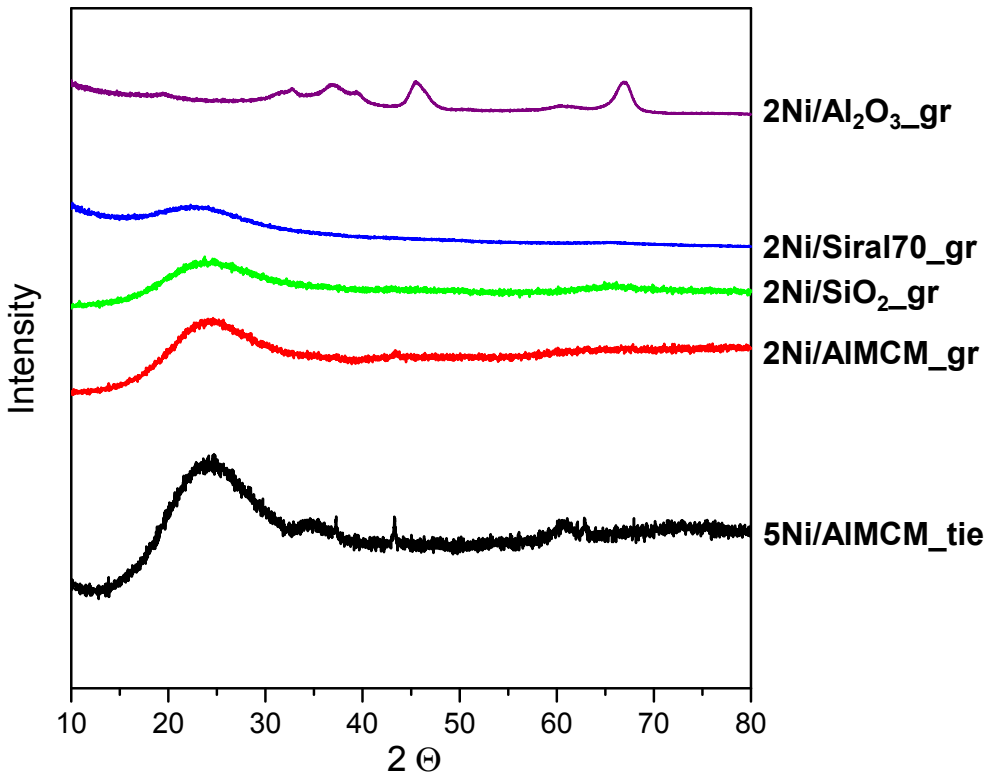

Figure S2 X-ray diffractograms of selected catalysts prepared by grafting of Ni acetyl acetonate (gr) or by template-ion exchange (tie)

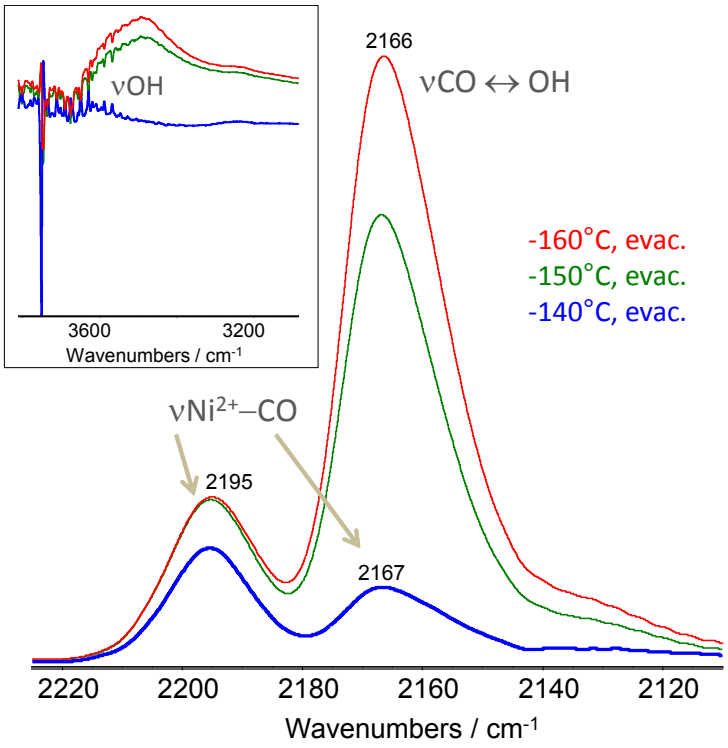

Figure S3 FTIR spectra of CO adsorbed on 2Ni/Siral/70_gr measured at different temperature after evacuation. Catalyst was pre-treated in air at 400 °C for 2 h before CO adsorption.

At -140°C no shifted νOH vibrations were detected around 3500 cm^{-1} so that we conclude the band at 2166 cm^{-1} stems not from νCO–OH but from νCO–Ni^{2+}. Therefore, this catalyst possesses two different Ni^{2+} species that adsorb CO (Bands at 2195 and 2167 cm^{-1}).

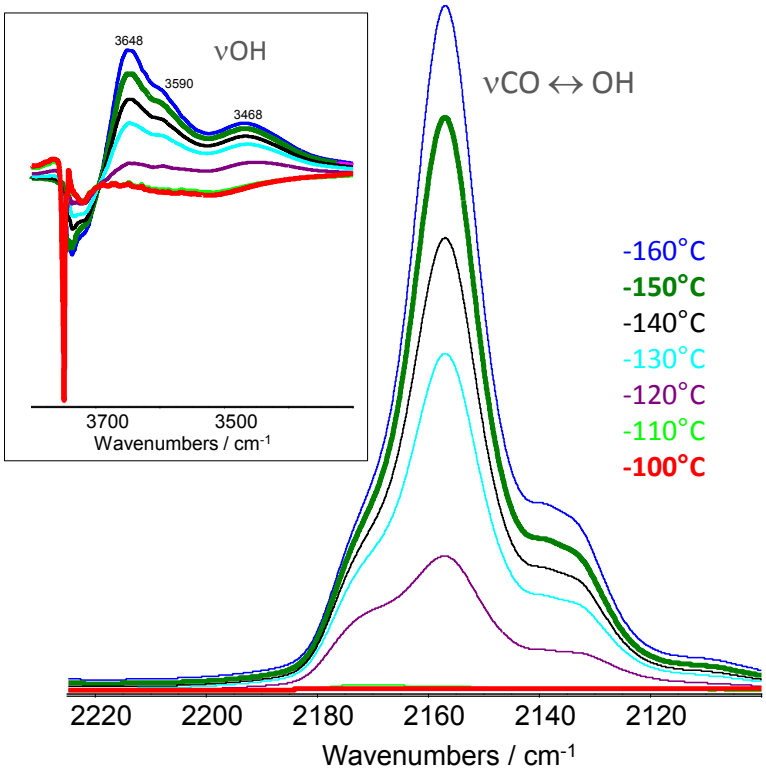

Figure S4 FTIR spectra of CO adsorbed on AlMCM-41 support measured at different temperature. Sample was pre-treated in air at 400 °C for 2 h before CO adsorption.

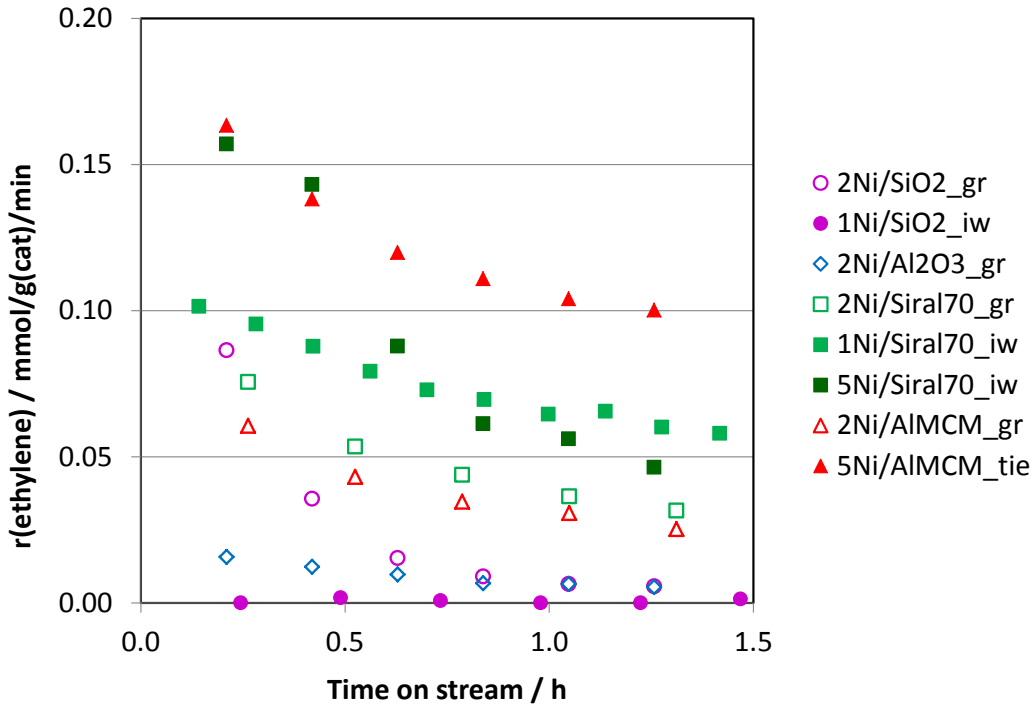

Figure S5 Ethylene conversion rates in EtP reaction over the different Ni-containing catalysts. Reaction conditions: Pre-treatment in air at 550°C for 2h, cooling down to reaction temperature of 375°C in N_2, flow rate of 17.5 ml·min^{-1} (10 vol % C_2H_4 in N_2), catalyst mass was 0.45g and 0.25g for samples with 1-2wt% Ni and 5wt% Ni, respectively.

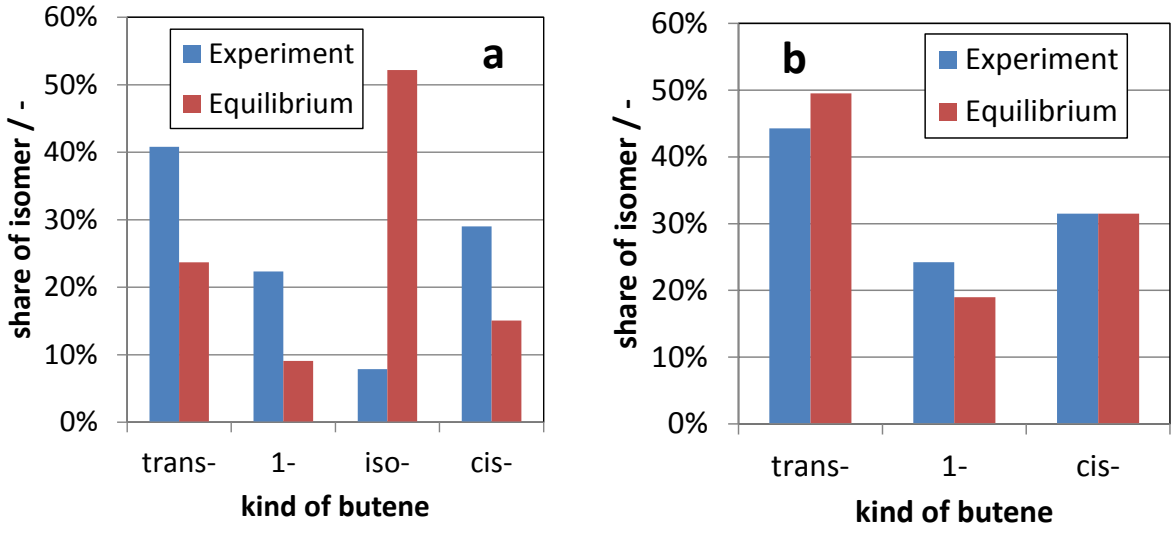

Figure S6 Experimental distribution of the different butenes formed over 2Ni/Siral70_gr compared to thermodynamic equilibrium. (a) all butenes, (b) only n-butenes

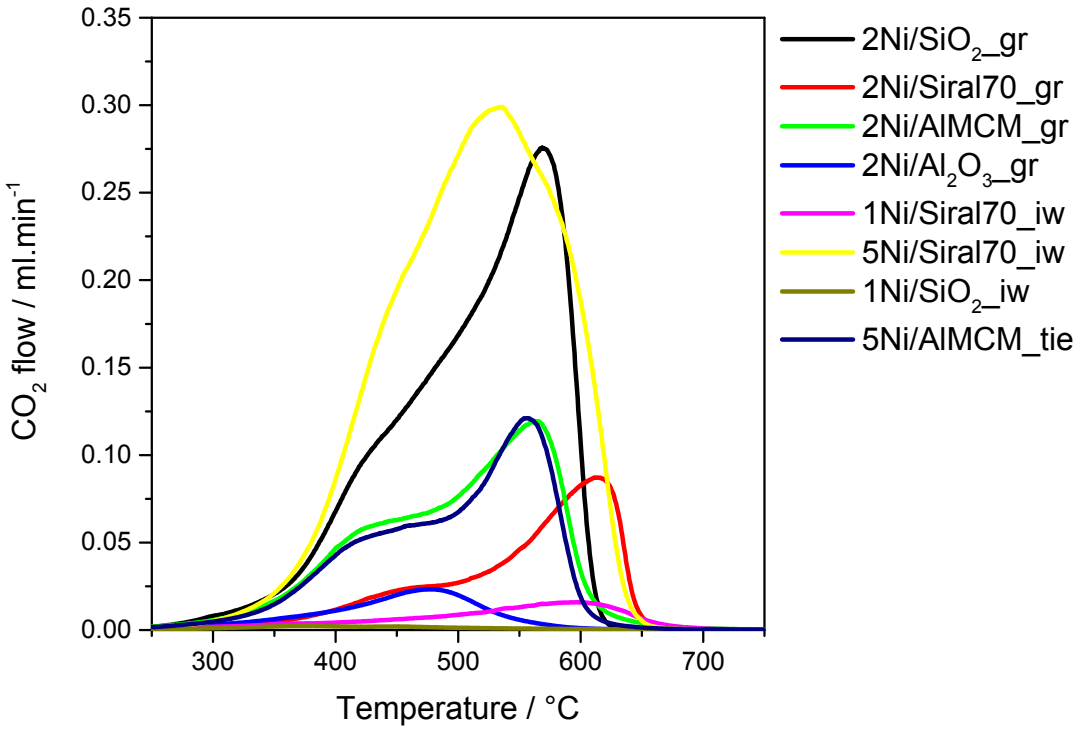

Figure S7 Temperature-programmed oxidation of coke deposited on supported Ni catalysts during EtP reaction. Conditions: 40 mg catalyst; heating with 10 °C·min^{-1} up to 1000 °C, gas flow rate of 10 ml·min^{-1} (5 vol% O_2 in Ar).