Electronic Supplementary Material (ESI) for Journal of Materials Chemistry This journal is © The Royal Society of Chemistry 2011

Supplementary Material (ESI) for Journal of Materials Chemistry This journal is (c) The Royal Society of Chemistry 2011

Synthesis of highly thermostable copper-nickel nanoparticles confined in the channels of ordered mesoporous SBA-15 silica

Adrian Ungureanu,^{*^a} Brindusa Dragoi,^a Alexandru Chirieac,^a Sébastien Royer,^b Daniel Duprez^b and Emil Dumitriu^a

^a Technical University Gheorghe Asachi of Iasi, Faculty of Chemical Engineering and Environmental Protection, 71A D. Mangeron Bd., 700050, Iasi, Romania, Fax: +40 - 232 271311, Tel: +40 - 232 278683; *E-mail: <u>aungureanu@tuiasi.ro</u> ^bUniversité de Poitiers, LACCO, UMR 6503 CNRS, 40, Av. du Recteur Pineau, 86022, Poitiers Cedex, France

Electronic Supplementary Information (ESI)

Experimental

Physico-chemical characterization

XPS analyses for calcined and in-situ reduced CuNi/SBA-15/500 sample (30 mL·min⁻¹, 5 vol. % H_2 in Ar at 350 °C for 5 h) were performed with a SSI X-probe (SSX-100/206) spectrometer from Surface Science Instrument. The analysis chamber was operated under ultrahigh vacuum with a pressure close to 5.10^{-9} Torr. X-rays were produced by a monochromatized aluminium anode working with monochromatic Al-K α (1486.6 eV) radiation (10 kV, 22 mA). For the measurements, the binding energy (BE) values were referred to the C 1s photopeak at 284.8 eV. The surface Cu/(Cu+Ni) atomic ratio was calculated by correcting the intensity with theoretical sensitivity factors based on Scofield cross sections. Peak decomposition was performed using 85% Gaussian and 15% Lorentzian types and a Shirley non-linear sigmoid-type baseline

Electronic Supplementary Material (ESI) for Journal of Materials Chemistry This journal is O The Royal Society of Chemistry 2011

Supplementary Material (ESI) for Journal of Materials Chemistry This journal is (c) The Royal Society of Chemistry 2011



Fig. S1. Normalised powder HAXRD patterns of CuNi/SBA-15 calcined at different temperatures.

Electronic Supplementary Material (ESI) for Journal of Materials Chemistry This journal is O The Royal Society of Chemistry 2011

Supplementary Material (ESI) for Journal of Materials Chemistry This journal is (c) The Royal Society of Chemistry 2011



Fig. S2. Typical EDX spectra for CuNi/SBA-15 calcined at 350 °C (a), 500 °C (b) and 600 °C (c).

b

с

a

Supplementary Material (ESI) for Journal of Materials Chemistry This journal is (c) The Royal Society of Chemistry 2011

Sample	Binding energy, eV						Cu/(Cu+Ni)
CuNi/SBA-15/500	Cu 2 <i>p</i> _{3/2}		Ni 2p _{3/2}		O 1s	Si 2p	atomic ratio
	Cu ²⁺	Cu ⁰	Ni ²⁺	Ni ⁰			
Before reduction	933.4 (916.9 ^a)	-	856.0	-	533.1	103.6	0.65
After reduction	-	932.6 (918.4 ^a)	856.1	852.6	533.1	103.7	0.61

Table S1. XPS binding energies obtained from curve-fitted values of experimental spectra for the sample CuNi/SBA-15/500 before and after reduction treatment at 350 $^{\circ}$ C

^ain brackets are the kinetic energies (KE) of the Auger Cu LMM transitions determined by Auger Electron Spectroscopy





(Reaction conditions: reduction temperature of 350 °C; 1ml trans-cinnamaldehyde; 25 ml PC as solvent; 0.265 g of catalyst; hydrogen flow of 1 L.h⁻¹; reaction temperature of 150 °C, agitation speed of 900 rpm. CNA conversions are reported after 60 min. of reaction. Selectivities are reported at isoconversion of ~ 20 mole % CNA)