Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2020

**Supporting Information** 

## Low temperature conversion of levulinic acid into γ-valerolactone using Zn to generate hydrogen from water and nickel catalysts supported on sepiolite

Adrián García<sup>a</sup>, Rut Sanchis<sup>a</sup>, Pablo J. Miguel<sup>a</sup>, Ana M. Dejoz<sup>a</sup>, María Pilar Pico<sup>b</sup>, María Luisa López<sup>c</sup>, Inmaculada Álvarez-Serrano<sup>c</sup>, Tomás García<sup>d</sup>, Benjamín Solsona<sup>a\*</sup>

<sup>a</sup> Departament d'Enginyeria Química, ETSE, Universitat de València, Av. Universitat, 46100 Burjassot, Valencia, Spain

<sup>b</sup> Sepiolsa, Avda. del Acero, 14-16, Pol. UP-1 (Miralcampo), 19200 Azuqueca de Henares, Spain

<sup>c</sup> Departamento de Química Inorgánica, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

<sup>d</sup> Instituto de Carboquímica (CSIC), C/Miguel Luesma Castán, 50018 Zaragoza, Spain

## **Experimental**

We have mentioned that in the tests undertaken with Zn the analyses of gases have detected the presence of hydrogen. This hydrogen in the gas phase can be quantified considering the free room of the flask employed in the experiments by knowing the proportion of hydrogen in the gas phase. As the free space in our three neck flasks is large compared to the reaction media we assume we are working at atmospheric pressure. Once we know the pressure of hydrogen in the gas-phase we can estimate the amount of H<sub>2</sub> dissolved in the liquid phase using the Henry's law equation:  $C_{H2}(\text{liquid}) = P_{H2}(\text{gas})/K_{\text{Henry}}$  being  $C_{H2}(\text{liquid})$  the concentration of hydrogen in the gas phase,  $P_{H2}(\text{gas})$  the partial pressure of H<sub>2</sub> in the gas over the liquid and  $K_{\text{Henry}}$  the Henry's constant. Overall, the hydrogen released during the experiments according to *Reaction 1* is used for the hydrogenation of LA but also a part is released into the gas phase and a small part remains dissolved into the liquid phase



Figure S1. GC-MS of a representative analysis showing the reactant and the main reaction product.



## Zoom between 8.5 and 16 min to identify minority products

Figure S2. GC-MS of a representative analysis between 8.5 and 16 min in order to identify minorities.



**Figure S3.** Effect of the Zn loading on the productivity to GVL usy4ning 2Ni/sep-ox catalyst. Reaction conditions: Zn loadings from 0 to 285 mg, remaining conditions in Experimental section.

**Table S1.** Summary of the measured  $d_{(hkl)}$  of used 2Ni/sep-ox + Zn in comparison with data cited in JCPDS database: files corresponding to hexagonal Zn and hexagonal ZnO, respectively.

d(hkl) (Å)	Possible structure	
2,8	ZnO 100	
2,6	ZnO 002	
2,47	ZnO 101	
2,39		Zn 002
2,14		
1,87	ZnO 102	Zn 101
1,71		
1,64	ZnO 110	Zn 102
1,2	ZnO 202	