- Supporting Information –

Filling Single-Walled Carbon Nanotubes with Lutetium Chloride: A Sustainable Production of Nanocapsules Free of Non-Encapsulated Material

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This Supporting Information has four pages and contains

five sections and four figures (Figs. S1- S4).

1. $LuCl_3$ complex with CPC/CAS

Aqueous solutions of 0.2 % (w/v) CPC and CAS were prepared, mixed in 1:1 ratio and diluted to $4\cdot10^{-3}$ %. A CPC/CAS solution (2 mL) was added to $LuCl_3$ aqueous solutions in the range of concentrations 10^{-2} to 10^{-8} M, keeping the final volume at 30 mL. Two different concentrations of CPC/CAS have been employed. From a qualitative point of view it is interesting to note that regardless of the concentration of CPC/CAS a royal blue color indicates the presence of lutetium chloride, not appreciable in the picture in b, and yellow indicates the absence of the metal salt (CPC/CAS in water has a yellow color). Greenish/reddish colors are observed between both stages.

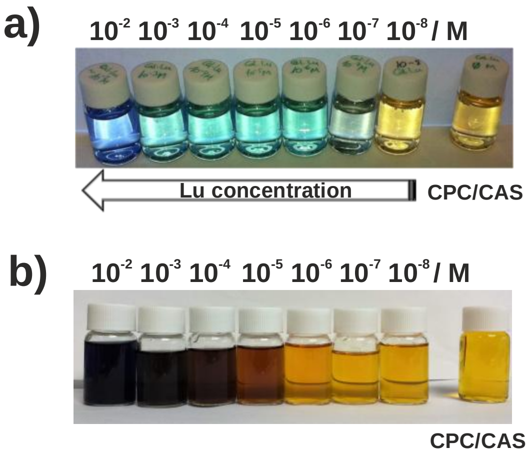

Figure S1. Vials containing 10^{-2}-10^{-8} M $LuCl_3$ in the presence of CPC/CAS showing a concentration-dependent change of color. A control sample of CPC/CAS is included on the right side of the photograph. The concentration of CPC/CAS is a) $4\cdot10^{-3}$% w/v and b) 0.2% w/v.

2. CPC/CAS test of the DSh protocol

Figure S2. Photos of aliquots after complexation with CPC/CAS using DSh for the removal of external $LuCl_3$ after first washing (left) and 4th final washing (right). The concentration of CPC/CAS is 0.2% w/v. Total volume of each fraction was 30 mL.

3. Additional HRTEM images of DSh sample

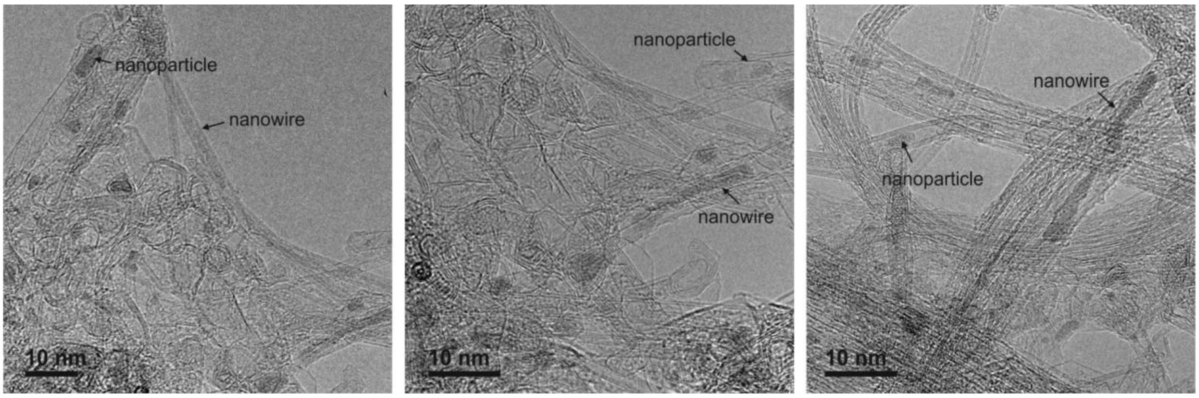

Figure S3. Additional HRTEM images of the sample of $LuCl_3$@SWCNTs after the final washing by the DSh protocol confirming that all the $LuCl_3$ is encapsulated within graphitic shells, as no external material is observed. Examples of small nanoparticles of $LuCl_3$ encapsulated within the CNTs as well as filling in the form of nanowires can be observed in the images.

4. EDX analyses on individual nanoparticles on DSh sample

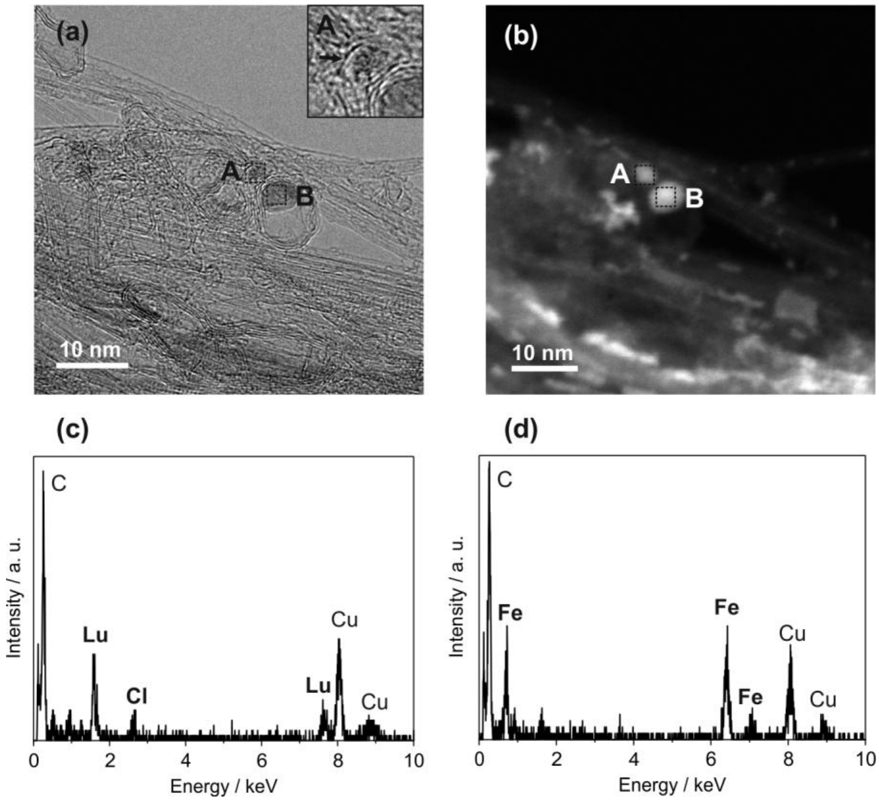

Figure S4. (a) HRTEM image on a bundle of CNTs showing nanoparticles **A** and **B** surrounded by graphitic shells. The inset shows nanoparticle **A** at higher magnification, with a black arrow pointing to the shell; (b) HAADF STEM images on the same area, where the nanoparticles appear with a bright intensity; (c) EDX analysis on nanoparticle **A** shows the presence of Lu and Cl, from the encapsulated material; (d) EDX analysis on nanoparticle **B** confirms that it is residual catalyst, as it is formed by Fe.

5. Calculation of filling yield[1]

Filling yield of $LuCl_3$@SWCNTs was calculated on the basis TGA residues in air: from empty nanotubes (R_1), clean filled nanotubes (R_2) and bulk material (R_A).

$$FY\ (wt\%) = \frac{100 \cdot (\mathrm{R}_2 - \mathrm{R}_1)}{\mathrm{R}_\mathrm{A} - \mathrm{R}_1}\ (1)$$

Bulk material (W_B) is product of oxidation of lanthanide halide (W_A), where x and y are stoichiometric coefficients of reaction and M is molar mass. Thus residue can be calculated according to following formula:

$$R_A = \frac{100 \cdot \mathrm{y} \cdot \mathrm{MW_B}}{\mathrm{x} \cdot \mathrm{MW_A}}\ (2)$$

1. Ballesteros, B.; Tobias, G.; Ward, M. A. H.; Green, M. L. H., Quantitative Assessment of the Amount of Material Encapsulated in Filled Carbon Nanotubes. *J. Phys. Chem. C.* **2009,** *113* (7), 2653-2656.