ELECTRONIC SUPPORTING INFORMATION

CHARGE TRANSFER IN STEAM PURIFIED ARC DISCHARGE SINGLE WALLED CARBON NANOTUBES FILLED WITH LUTETIUM HALIDES.

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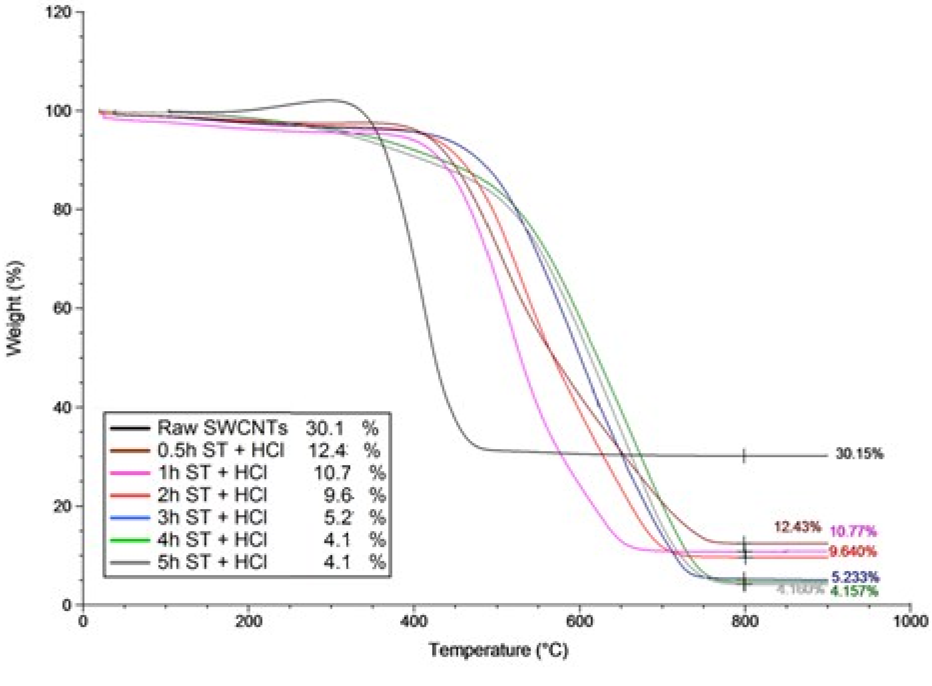

Figure ESI1: TGA curves of raw SWCNTs and steam treated (ST) SWCNTs for different periods of time (after an HCl wash). Measurements were performed in air with a heating ramp of 10 ºC/min. Numbers in the legend correspond to the inorganic solid residue obtained at 900 º C (in wt.%).

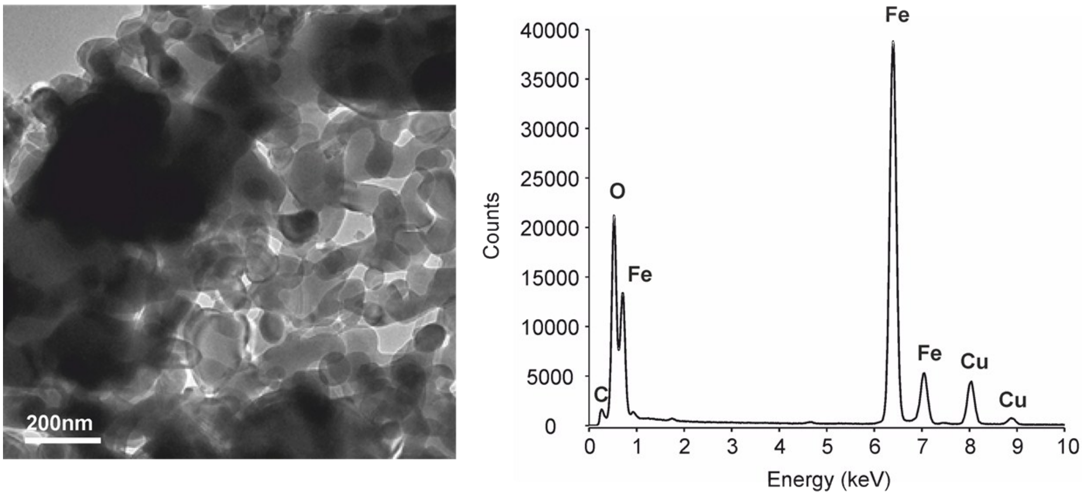

Figure ESI2: Energy dispersive X-ray spectrum (EDX) of the TGA residue obtained after the complete combustion of the raw SWCNTs (TGA performed under air at 10 ºC/min until 900 ºC). The micrograph shows a transmission electron microscopy (TEM) image of the analyzed area. Analyses were performed on an FEI Tecnai G2 F20 TEM. The sample was deposited on a lacey carbon coated copper grid. Therefore carbon and copper signals can be assigned to the support and thus the residue would contain iron and oxygen.

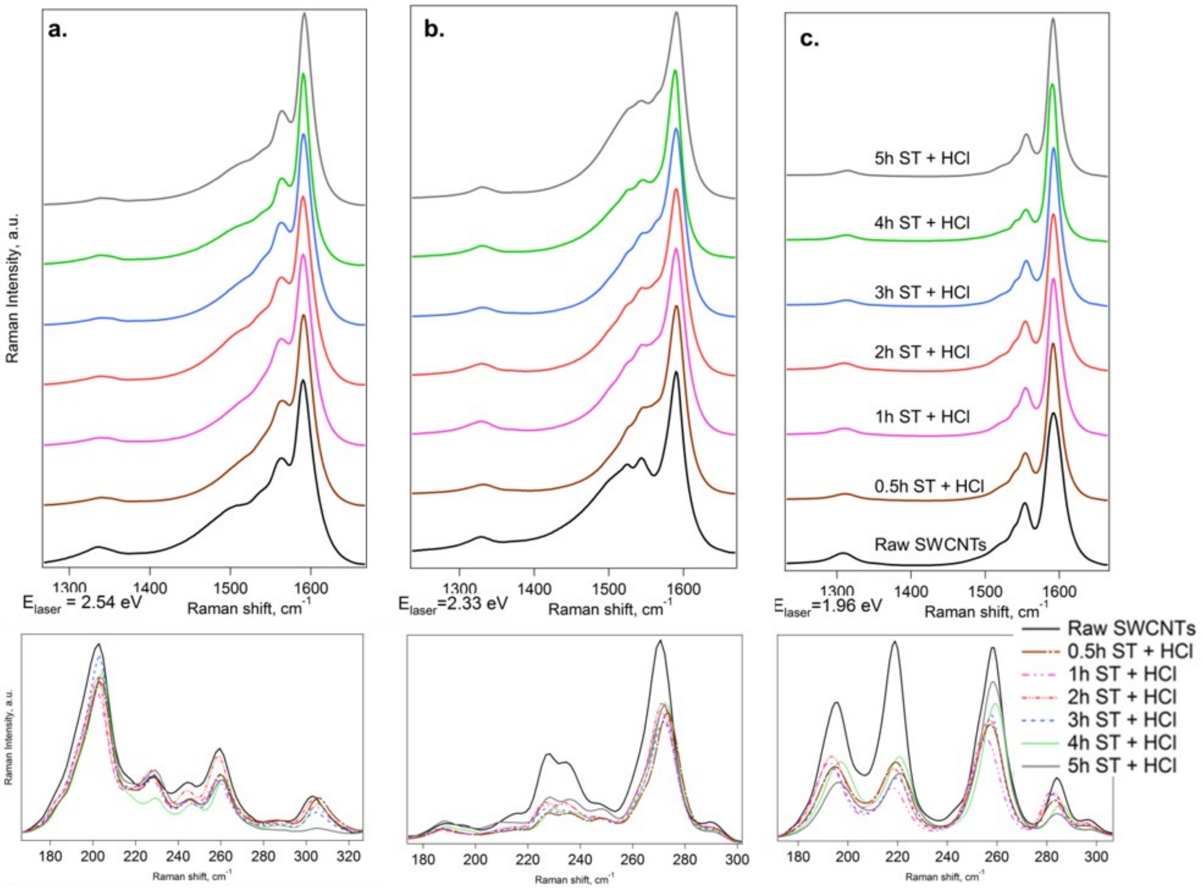

Figure ESI3: Resonance Raman spectra D and G-band region and the RBM region on the bottom, of raw SWCNTs and steam treated SWCNTs for different periods of time (after an HCl wash), excited by different laser lines a. 2.54 eV (488 nm), b. 2.33 eV (532 nm) and c. 1.96 eV (633 nm). Each spectrum is an average based on 900 (1.96 eV) and 49 spectra (2.33 and 2.54 eV) measured in different points. The spectra are offset for clarity.

On the bottom of the Figure ESI3, the RBM region of the Raman spectra of the raw SWCNTs and steam treated SWCNTs for different energy excitation used (a. 2.54, b. 2.33 and c. 1.96 eV) is observed. No remarkable changes are perceived, probing that the nanotube structure is preserved. The bands at low frequency transition, which correspond to nanotubes with large diameters, present a small decrease in intensity. Consequently, mainly nanotubes with large diameter seem to be affected by the probed treatments. The G-band spectra are typical for CNTs bundles where the widths of the G-band are about 20 cm^{-1} (isolated nanotubes display smaller widths) and are centered at 1590 cm^{-1}. The broadening of the G-band indicates that semiconducting and metallic carbon nanotubes are in resonance at the used laser excitation energies. The D-band appears at 1337, 1330 and 1310 cm^{-1} using 2.54, 2.33 and 1.96 eV as excitation energy, respectively, since the frequency of the D-band is laser energy dependent.

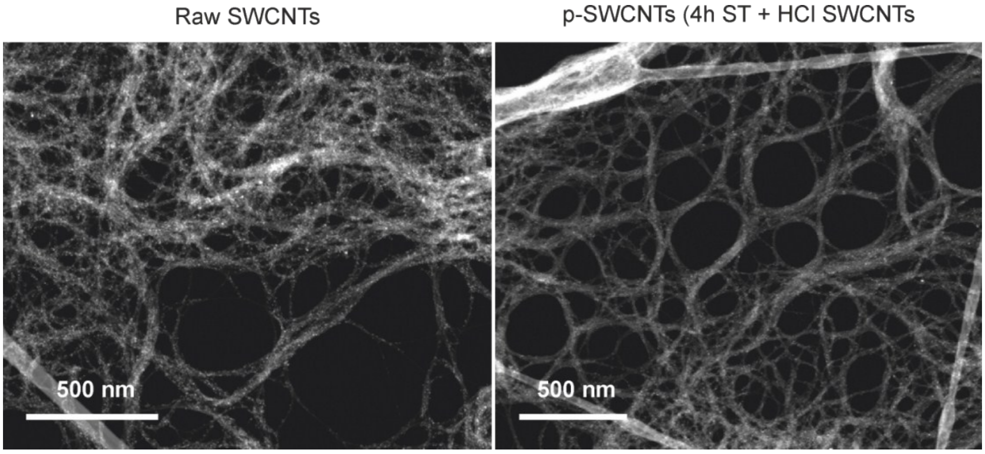

Figure ESI4: Scanning transmission electron microscopy images of raw SWCNTs and the 4h steam treated SWCNTs (after an HCl wash).

The length distribution of the samples was determined from an analysis of scanning electron microscope (SEM) images using Digital Micrograph software. The sample for SEM observation was prepared as follows: first, a tiny amount of nanotubes was sonicated in 3 mL of *ortho*-dichlorobenzene (Sigma-Aldrich, 99%) between 30 to 45 min to achieve a good dispersion (the suspension presented a homogeneous grey colour). Then, about 10 drops of this dispersion were placed onto a copper grid coated with a carbon film and left to dry. SEM studies were carried out on an FEI Magellan 400L XHR using an In-Lens Detector (TLD) at 2 kV. In these conditions, surface-sensitive images with spatial resolution below 1 nm are obtained, allowing the visualization of individual SWCNTs. [1] Two hundred isolated SWCNTs were measured to determine the length distribution of the raw SWCNTs as well as the 4 h steam and HCl-treated CNTs (pSWCNTs).

Both raw arc-discharge SWCNTs and pSWCNTs were dispersed and characterized using SEM to determine the length of individual nanotubes. Statistical analysis was performed with a sample size of 200 for each of the groups, namely, control group (raw SWCNTs) and pSWCNTs. The resulting histograms are presented in Figure ESI5. In contrast to CVD-grown nanotubes, where a 4 h steam treatment results in over a 40% decrease in the median length distribution of the sample, a much smaller effect is observed on arc-discharge nanotubes after the same treatment time. The median length distribution of raw arc-discharge SWCNTs (537 nm) is reduced to 457 nm after 4 h steam (and HCl) which corresponds to a 15% reduction. This indicates a completely different reactivity of the nanotubes towards steam depending on their source.

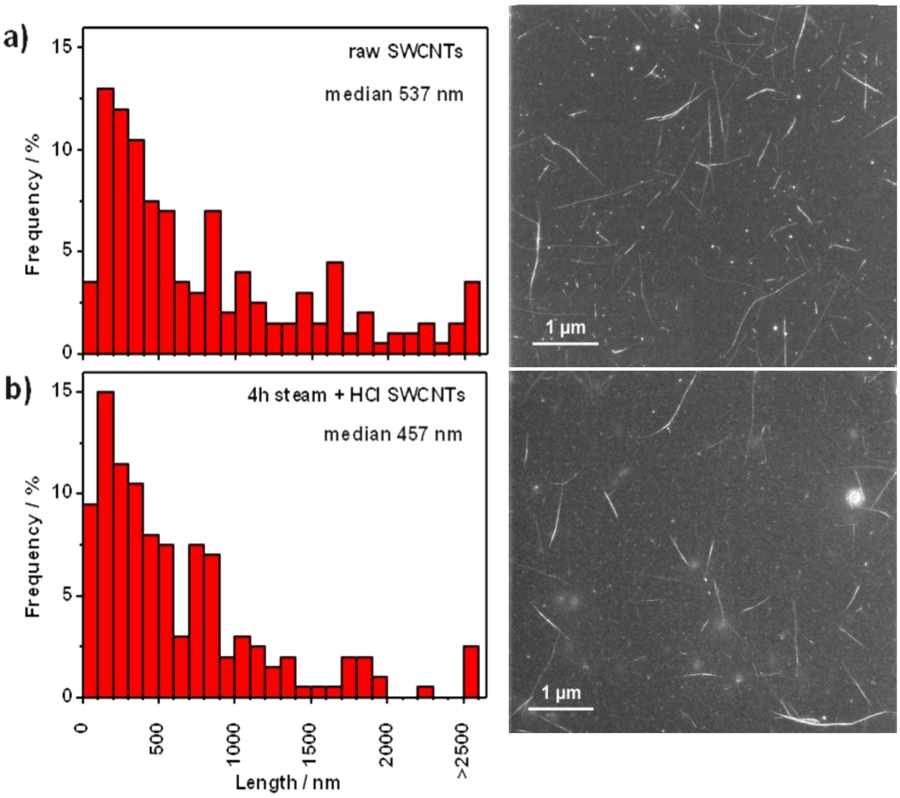

Figure ESI5: Histograms representing the length distribution of the a) raw SWCNTs and b) the 4h steam treated SWCNTs (after an HCl wash). For each sample 200 individual nanotubes were measured. Representative SEM images are included on the right.

EDX spectra were acquired at 20 kV on an FEI Quanta 650FESEM coupled to an Oxford Instruments XMax20 EDX detection system or on an FEI Tecnai G2 F20 TEM operated at 200 kV equipped with an EDX super ultra-thin window (SUTW) X-ray detector. STEM images were acquired with an FEI Magellan 400L XHR SEM operated at 20 kV with a high-angle annular dark-field (HAADF) detector. For TEM and HAADF-STEM imaging, the samples of LuX_3@pSWCNTs (X = Cl, Br, I) were dispersed in ethanol and a few drops were deposited onto lacey carbon-coated copper grids. In the case of EDX analyses in the Quanta 650 FEG SEM, the samples were dispersed in ethanol and deposited dropwise onto Si chip supports.

The filling yield was calculated as $FY(wt\%) = \frac{g_{LuX3}}{g_{LuX3} + g_C} \times 100$,

where g_{LuX3} is the amount of the corresponding lutetium(III) halide (LuX_3) and g_C is the amount of carbon (pSWCNTs), both represented in weight percentage. These values were extracted from quantification of EDX analyses, averaging 16–18 spectra for each sample, namely $LuCl_3$@pSWCNTs, $LuBr_3$@pSWCNTs and LuI_3@pSWCNTs.

EDX analysis reveals the presence of $LuCl_3$, $LuBr_3$ and LuI_3 in the samples. The filling yield was calculated by analysing 16–18 EDX/SEM spectra of LuX_3@pSWCNTs (X = Cl, Br, I) samples and turned out to be: $LuCl_3$@pSWCNTs = 7.1 wt%, $LuBr_3$@pSWCNTs = 9.8 wt% and LuI_3@pSWCNTs = 7.8 wt%.

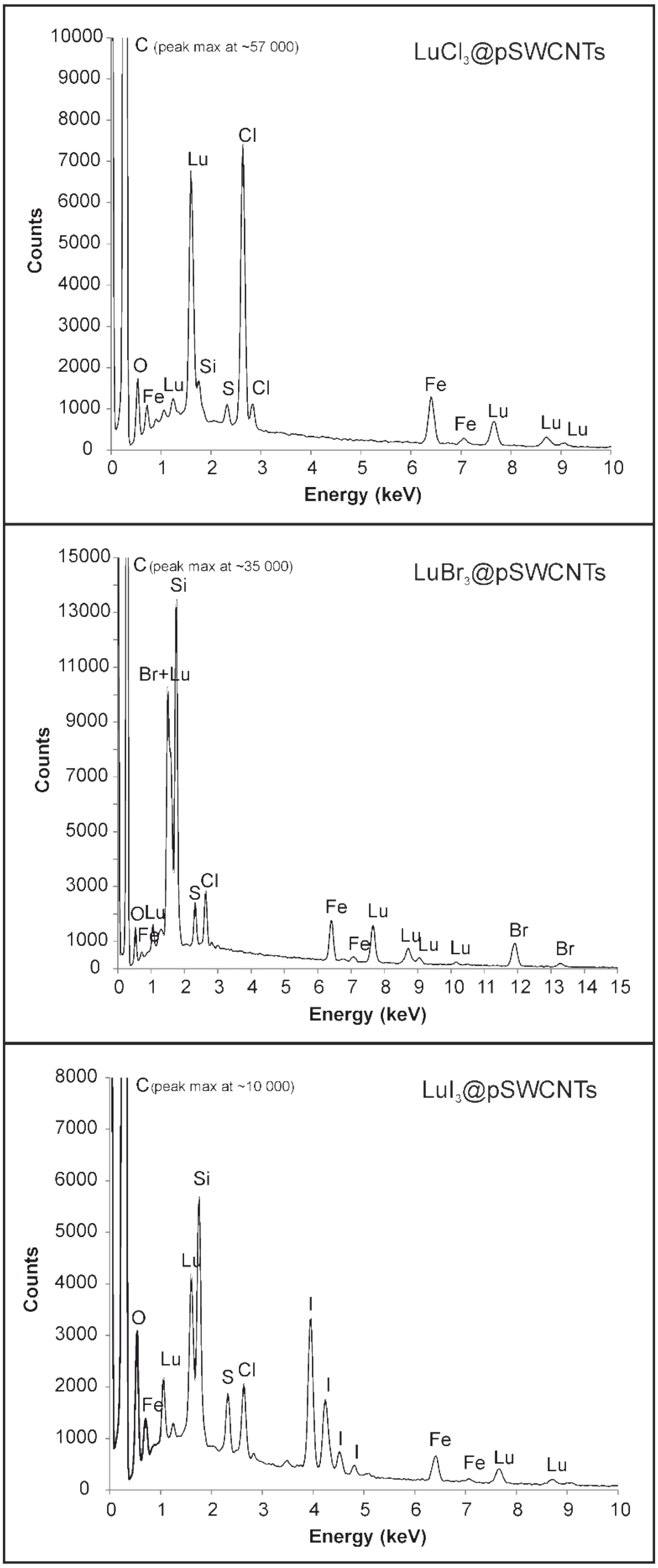

Figure ESI6: Energy dispersive X-ray spectra (EDX) of LuCl$_3$@pSWCNTs, LuBr$_3$@pSWCNTs and LuI$_3$@pSWCNTs. Analyses were performed on a FEI Quanta 650FESEM. The samples were deposited onto Si chip supports.

Table ESI1: Raman frequency of the most intense RBM bands and their assignment of the electronic transitions using the Kataura plot for the pSWCNTs and $LuCl_3$@pSWCNTs, $LuBr_3$@pSWCNTs and LuI_3@pSWCNTs samples acquired at different laser excitation wavelenghts.

	2.54 eV				**2.33 eV**		**1.96 eV**			
	Raman shift, cm^{-1}				**Raman shift, cm^{-1}**		**Raman shift, cm^{-1}**			
	E_{33}^S	E_{11}^M	E_{11}^M	E_{22}^S	E_{22}^S	E_{11}^M	E_{11}^M	E_{11}^M	E_{22}^S	E_{22}^S
pSWCNTs	203	227	260	305	188	272	196	219	257	283
$LuCl_3$@pSWCNTs	201	226	258	303	188	272	198	217	255	281
$LuBr_3$@pSWCNTs	203	227	248	303	189	274	197	220	258	283
LuI_3@pSWCNTs	205	227	256	-	-	274	200	221	258	-

Table ESI2: Raman frequency of the G-band in the Raman spectra of the pSWCNTs and $LuCl_3$@pSWCNTs, $LuBr_3$@pSWCNTs and LuI_3@pSWCNTs samples acquired at different laser excitation wavelenghts.

	E_{laser}, eV	**$G^{-}_{metallic}$, cm^{-1}**	**$G^{-}_{semiconducting}$, cm^{-1}**	**G^{+}, cm^{-1}**
pSWCNTs	**1.96**	1540	1554	1591
$LuCl_3$@pSWCNTs		1531	1550	1588
$LuBr_3$@pSWCNTs		1534	1555	1592
LuI_3@pSWCNTs		1534	1557	1593
pSWCNTs	**2.33**	1526	1560	1590
$LuCl_3$@pSWCNTs		1525	1556	1590
$LuBr_3$@pSWCNTs		1526	1558	1592
LuI_3@pSWCNTs		1521	1559	1592
pSWCNTs	**2.54**	1532	1561	1591
$LuCl_3$@pSWCNTs		1530	1557	1589
$LuBr_3$@pSWCNTs		1532	1559	1591
LuI_3@pSWCNTs		1539	1559	1592

Table ESI3: Raman frequency of the D-band in the Raman spectra of the pSWCNTs and LuX_3@pSWCNTs (X= Cl, Br, I) samples acquired at different laser excitation wavelenghts.

	E_{laser}, eV	**D, cm^{-1}**
pSWCNTs	**2.54**	1337
$LuCl_3$@pSWCNTs		1339
$LuBr_3$@pSWCNTs		1344
LuI_3@pSWCNTs		1347
pSWCNTs	**2.33**	1330
$LuCl_3$@pSWCNTs		1332
$LuBr_3$@pSWCNTs		1336
LuI_3@pSWCNTs		1338
pSWCNTs	**1.96**	1310
$LuCl_3$@pSWCNTs		1307
$LuBr_3$@pSWCNTs		1313
LuI_3@pSWCNTs		1316

References

1) S. Sandoval, M. Kierkowicz, E. Pach, B. Ballesteros, G. Tobias. *MethodsX* 5 (2018) 1465–1472