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Supplementary Information for:

Design and characterization of functionalized silica nanocontainers for self-healing materials

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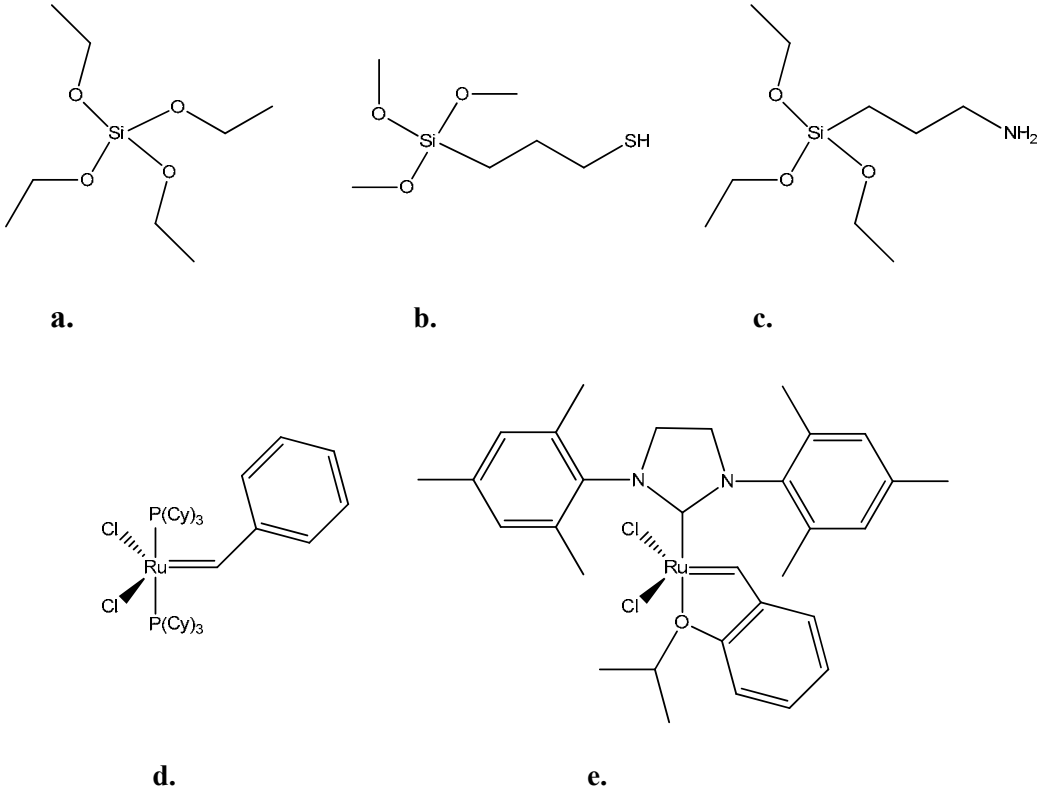
Chemical structures of the reagents



a. **b.** **c.**

d. **e.**

Fig. S1 Chemical structures of **a:** tetraethoxysilane (TEOS), **b:** 3-mercaptopropyltrimethoxysilane (MPTMS), **c:** 3-aminopropyltriethoxysilane (APTES), **d:** Grubbs´ catalyst 1st generation, **e:** Hoveyda-Grubbs' catalyst 2nd generation.

Non-functionalized nanocapsules with DCPD in the core

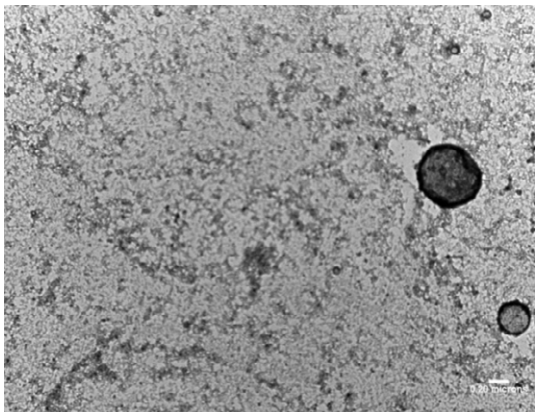
Influence of the amount of the liquid core

The nanocapsules synthesis followed the procedure reported in the experimental part with the exception of the amounts of hexadecane and DCPD (Table S1).

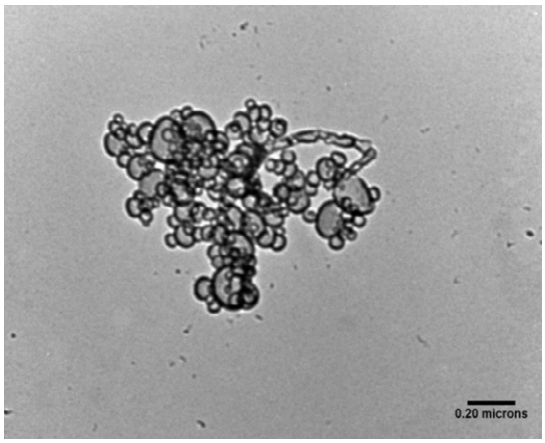
Table S1. Composition of the nanocapsules prepared with different amount of liquid core.

Entry	HD [g]	DCPD [g]	D_h * [nm]	PDI * [%]
JF41-3	0	0.66	810	20
JF68-1	0.5	0.5	160	50
JF68-2	0.75	0.75	170	40
JF68-3	1.0	1.0	190	40
JF68-4	2.0	2.0	240	40

* measured by DLS



a.



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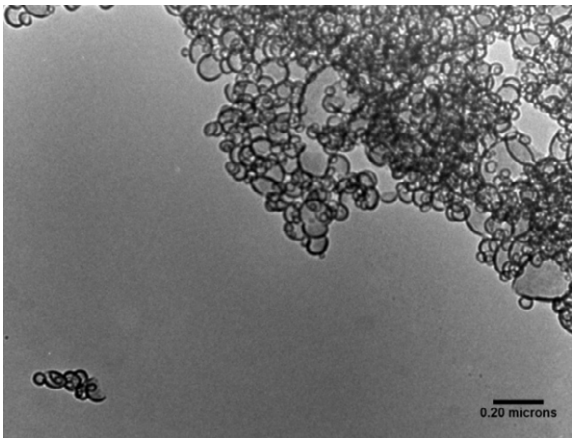

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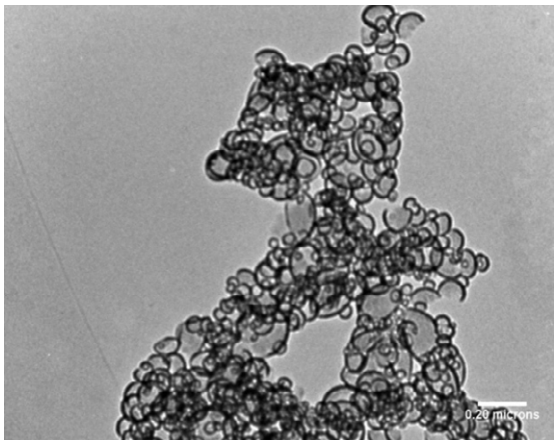

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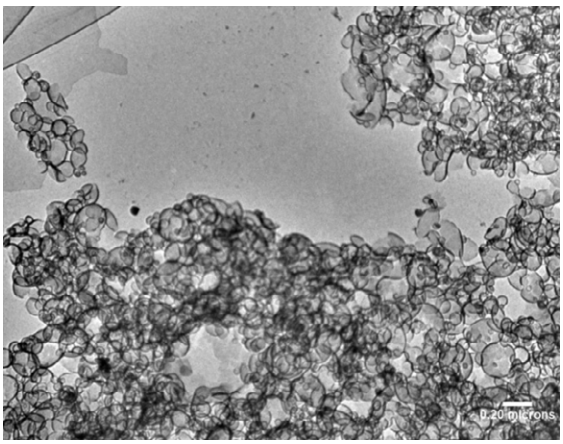


e.

Fig. S2 TEM micrographs of the samples prepared with **a:** only DCPD as liquid core (JF41-3); and different amounts of liquid core (50 wt.% DCPD in HD) **b:** 1 g (JF68-1), **c:** 1.5 g (JF68-2), **d:** 2 g (JF68-3), and **e:** 4 g (JF68-4).

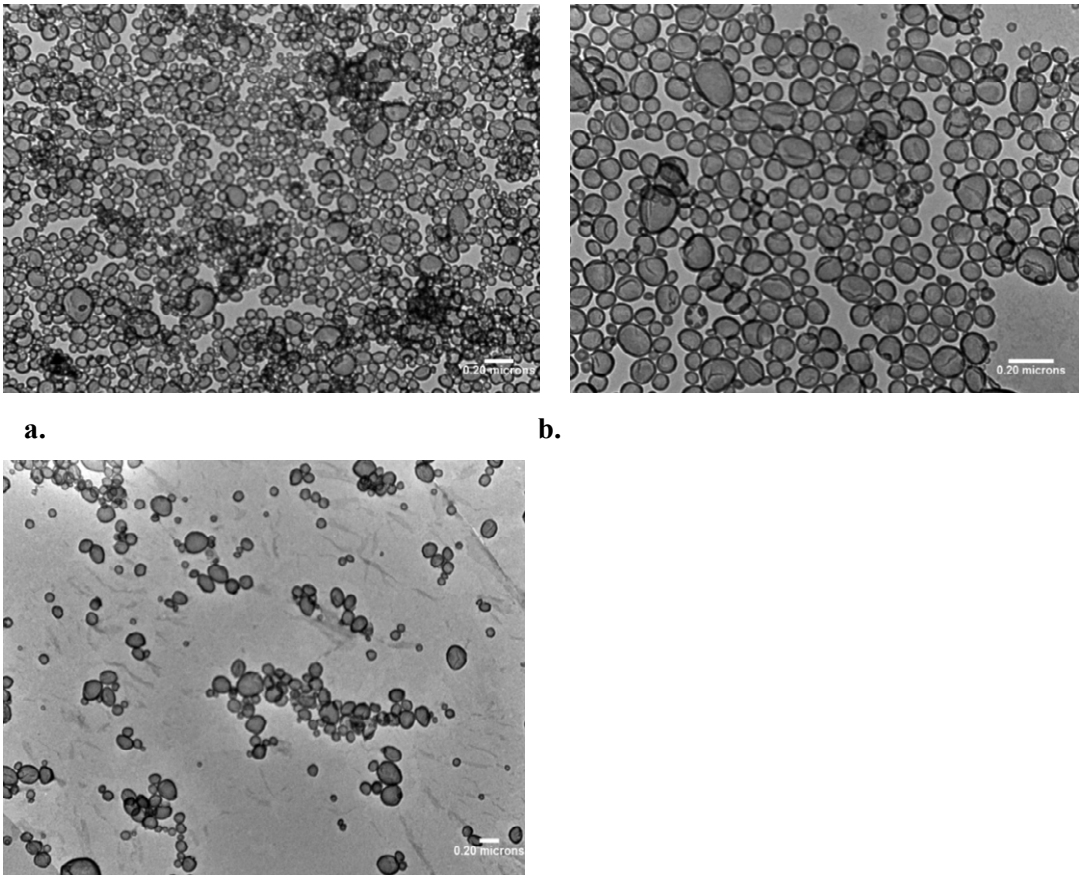
Influence of the amount of dispersed phase

Some nanoparticles were prepared with higher amounts of the mixture TEOS/HD/DCPD, the ratio (TEOS:HD:DCPD) of 6:1:1 (wt.) being kept constant (Table S2).

Table S2. Composition of the nanocapsules prepared with increasing amount of dispersed phase.

Entry	HD [g]	DCPD [g]	TEOS [g]	dispersed phase [wt.%]	D_h * [nm]	PDI * [%]
JF41-2	0.33	0.33	2.0	8.1	140	50
JF70-1	0.50	0.50	3.0	11.8	170	20
JF70-2	0.66	0.66	4.0	15.1	230	30
JF70-3	1.00	1.00	6.0	21.0	250	40

* measured by DLS



a. **b.**

c.

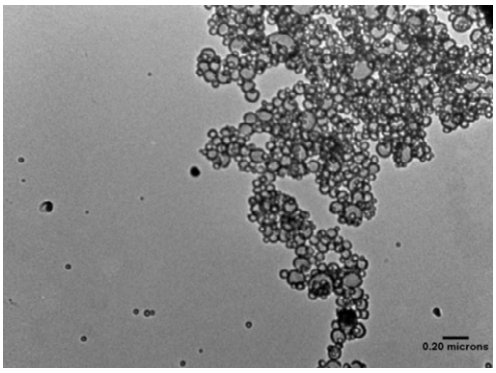
Fig. S3 TEM micrographs of the samples prepared with different amounts of the dispersed phase. **a:** 11.8 wt.% (JF70-1), **b:** 15.1 wt.% (JF70-2), **c:** 21.0 wt.% (JF70-3).

Influence of the surfactant

The amount of surfactant in the miniemulsions was varied to obtain different sizes for the nanocapsules (Table S3).

Table S3. Composition of the nanocapsules prepared with increasing amount of dispersed phase.

Entry	HD	DCPD	TEOS	H_2O	CTMA-Cl	D_h *	PDI *
	[g]	[g]	[g]	[g]	[mg]	[nm]	[%]
JF41-2	0.33	0.33	2.0	30	23	140	50
JF69-1	0.33	0.33	2.0	30	15	160	50
JF68-2	0.33	0.33	2.0	30	10	870	60
JF91-1	0.5	0.5	3.0	15	10	280	40
JF91-2	0.5	0.5	3.0	15	8	340	40
JF91-3	0.5	0.5	3.0	15	6	410	20



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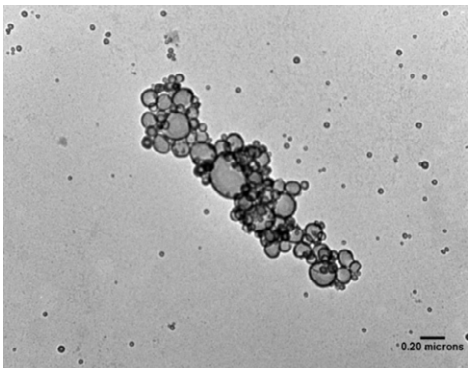

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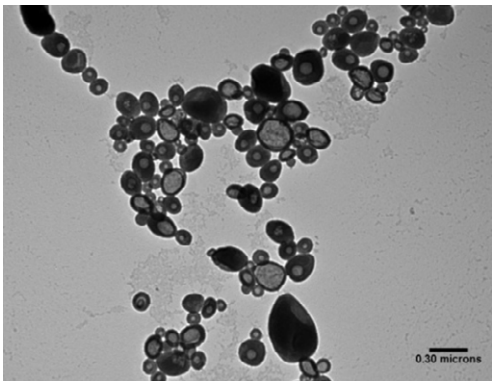
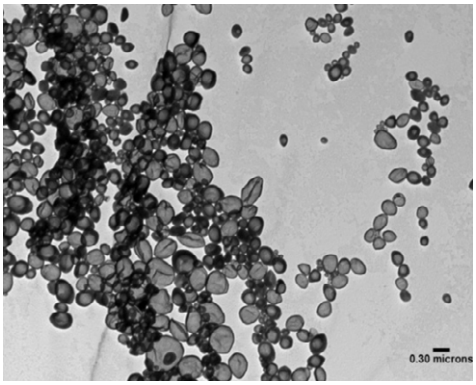


c.

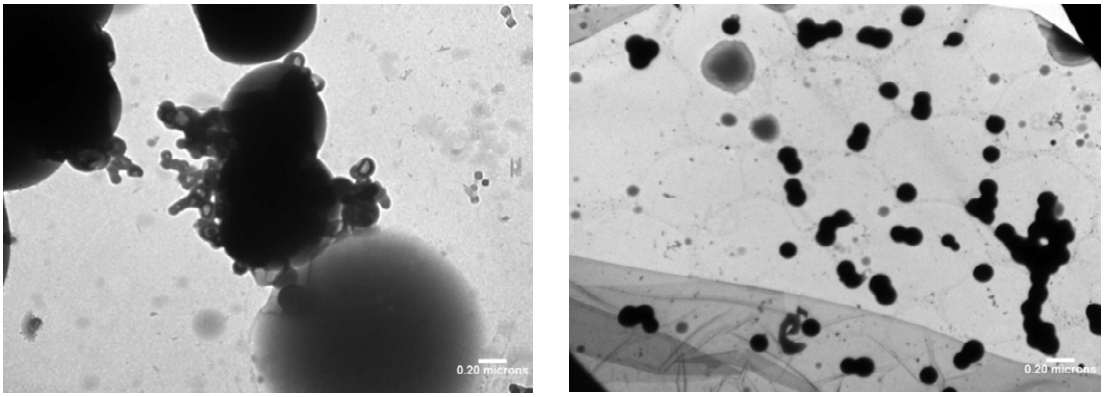


d.

Fig. S4 TEM micrographs of the samples prepared with different amount of surfactant **a:** JF69-1, **b:** JF68-2, **c:** JF91-2, **d:** JF91-3.

Addition of MPTMS

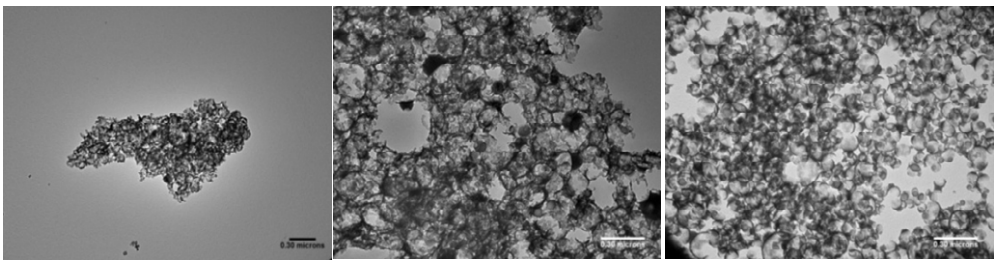
Some experiments were performed according to the experimental part but using MPTMS as sole alkoxysilane with either a 50 wt.% solution of DCPD in HD (JF56-2, D_h = 120 ± 50 nm), or only HD (JF56-3, D_h = 200 ± 80 nm) as liquid core. In both cases, only nanoparticles were obtained (see Fig. S4).



a. **b.**

Fig. S5 TEM micrographs of the samples prepared with different amount of surfactant **a:** JF56-2, **b:** JF56-3.

Addition of APTES



a. **b.** **c.**

Fig. S6 TEM micrographs of the samples prepared with 5 wt.% APTES added **a:** directly after sonication, **b:** 1 h after, **c:** 2.5 h after sonication.

EDX measurements

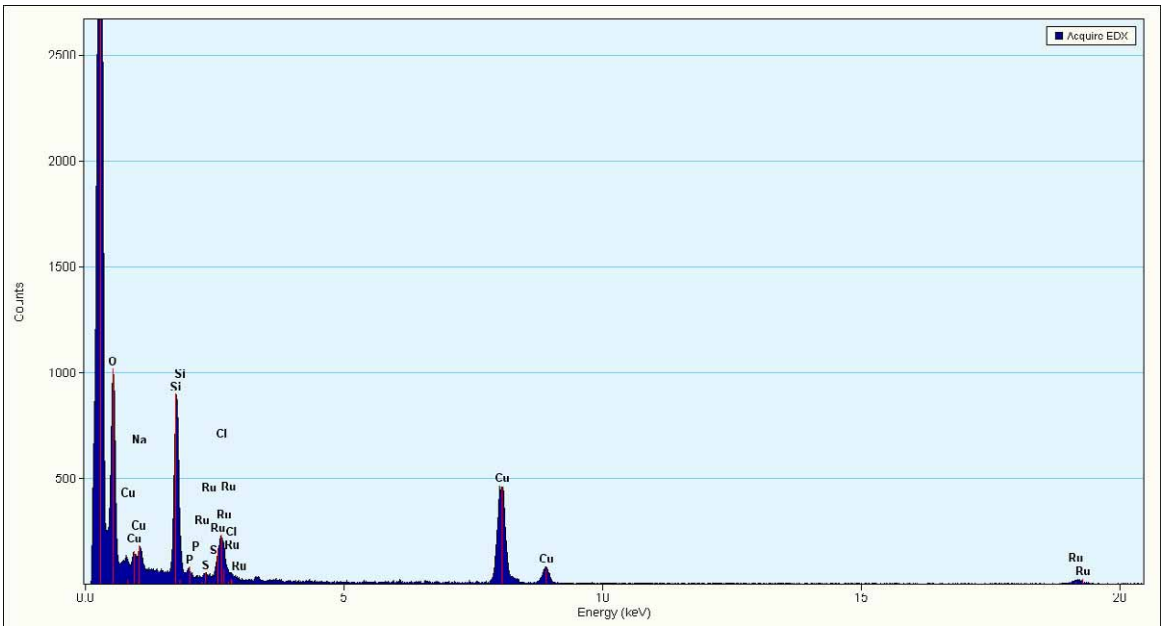


Fig. S7 EDX spectrum of the silica nanocaspule encapsulating the Grubbs' catalyst. Ruthenium could be detected.

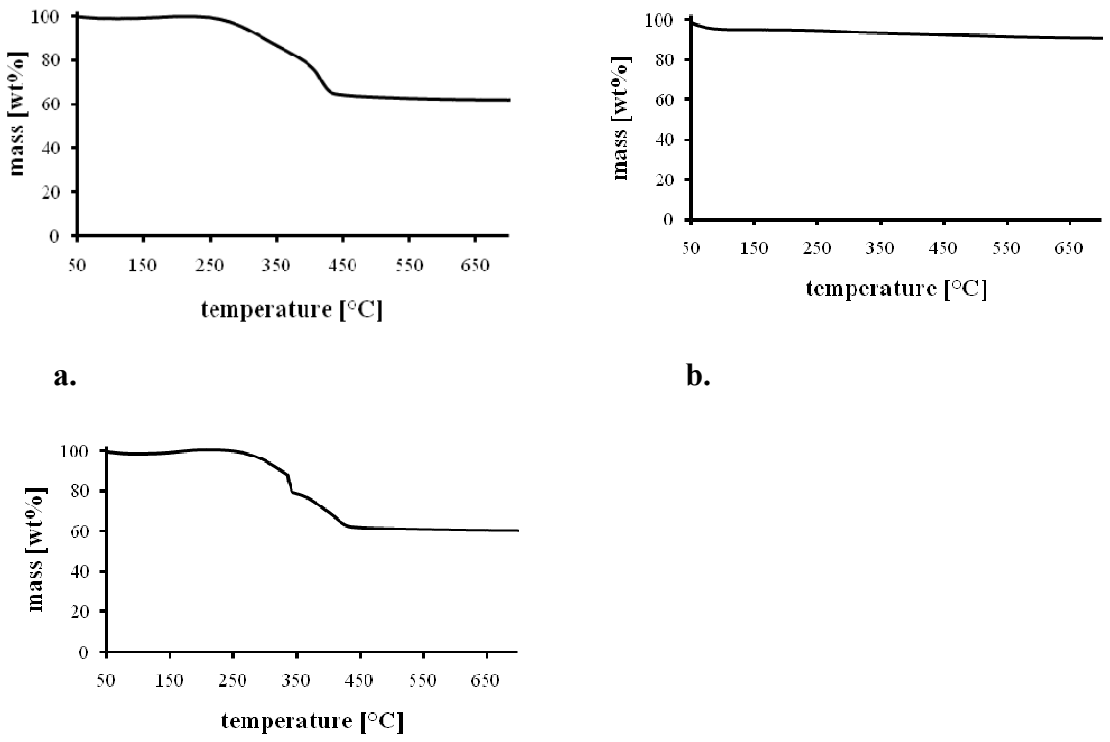


Fig. S8 TGA thermograms of freeze-dried samples **a:** SH2; **b:** sample JF139-5 (DCPD capsules, **c:** SH3.