

# Supplementary materials : An Electro-Elastic Theory for the Mechanically Assisted Photo-excitation in Core-Shell Spin-Crossover Nanoparticles

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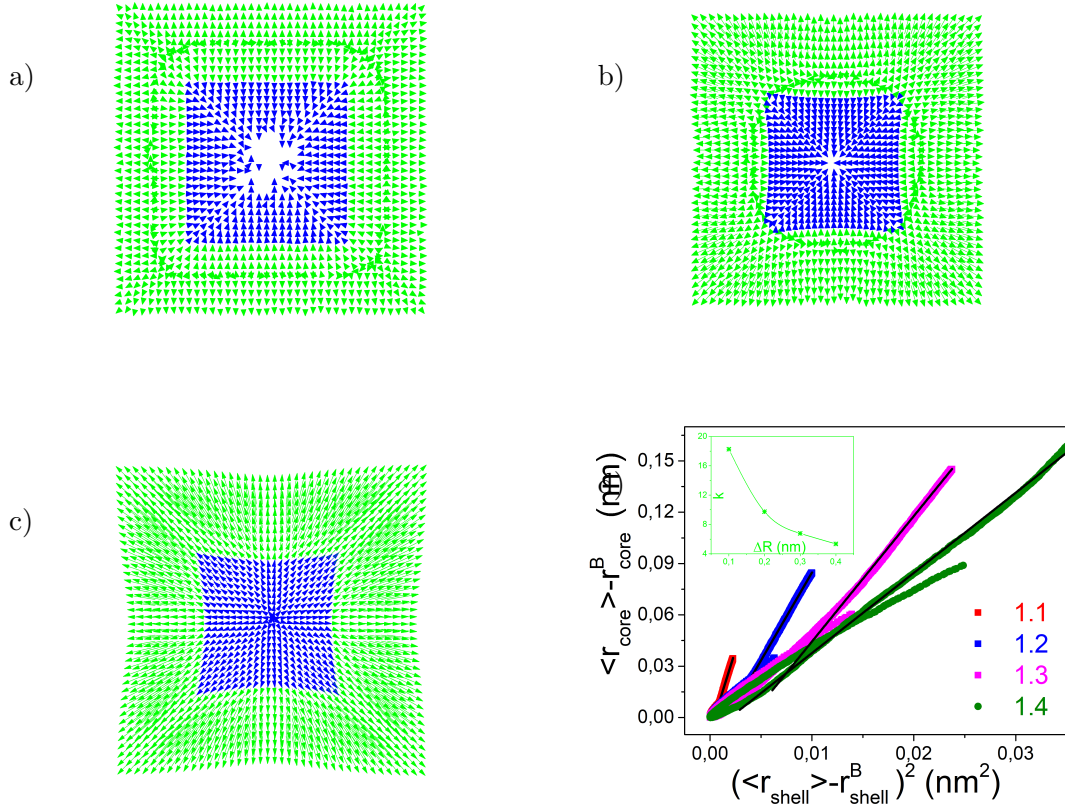


Fig. SM1: The displacement field corresponding to the points A (a), C (b) of the cure  $\langle r \rangle_{core}$  (Fig.2 (b) (bottom)) and at the mechanical equilibrium (c). Green (blue) arrows correspond to the shell (core). (d)  $(\langle r \rangle_{core} - r_{core}^B)$  as a function of  $(\langle r \rangle_{shell} - r_{shell}^B)^2$  for the different  $R_{shell}$ . Inset: The average rate of mechanical change,  $k$ , as a function of the misfit  $\Delta R$ .

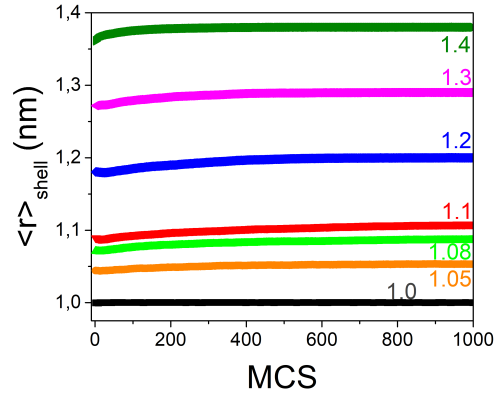


Fig. SM2: Shell's lattice parameter through the photoexcitation process.

Fixed <u>nn</u> bonds (nm)			Varied lengths (nm)	Calculated <u>nn</u> bonds (nm) and HS <u>fraction</u>				
$R_{shell}$	$R_{core}^{HS}$	$R_{core}^{LS}$		<i>After mechanical relaxation and before photoexcitation</i>		<i>After photoexcitation</i>		
$R_{shell}$	$R_{core}^{HS}$	$R_{core}^{LS}$	$R_{shell}$	$R_{core}^{LS}$	$R_{shell}$	$R_{core}^{HS}$	$R_{shell}$	$^{HS}$ fraction(%)
1.0	1.2	1.0	1.0	1.0	1.0	–	1.0	0
1.1	1.2	1.0	1.1	1.02	1.089	1.17	1.12	90
1.2	1.2	1.0	1.2	1.048	1.18	1.2	1.2	100
1.3	1.2	1.0	1.3	1.083	1.273	1.225	1.29	100
1.4	1.2	1.0	1.4	1.121	1.366	1.25	1.38	100

Table 1: Summary of the fixed, varied and calculated lattice parameters and HS fraction from Monte-Carlo simulations of the core-shell nanoparticle.

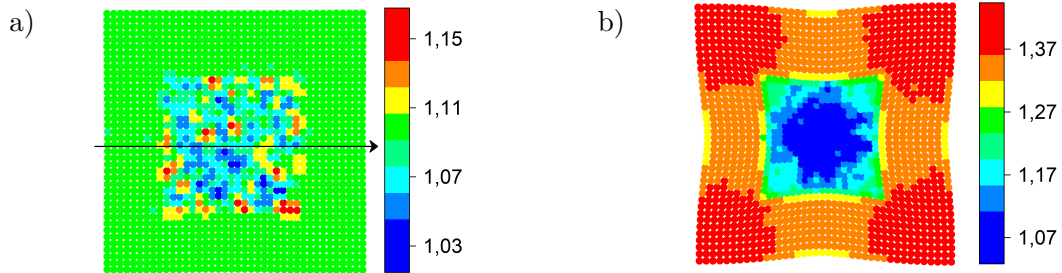


Fig. SM3: Map of the nearest neighbors intermolecular bond lengths over the nanoparticle corresponding to the lattice configuration shown in Fig. 5 (a), whose  $R_{shell}$  are 1.1 nm (a) and 1.4 nm (b)

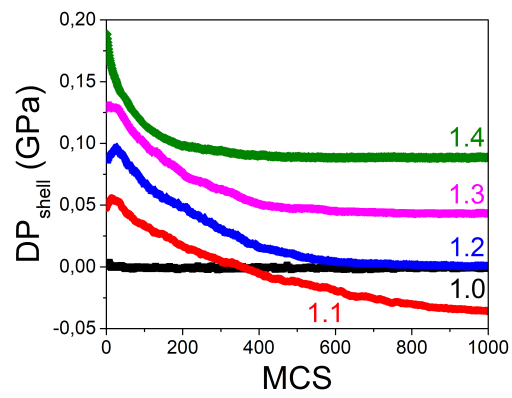


Fig. SM4: The density of pressure in the shell through the photoexcitation process.

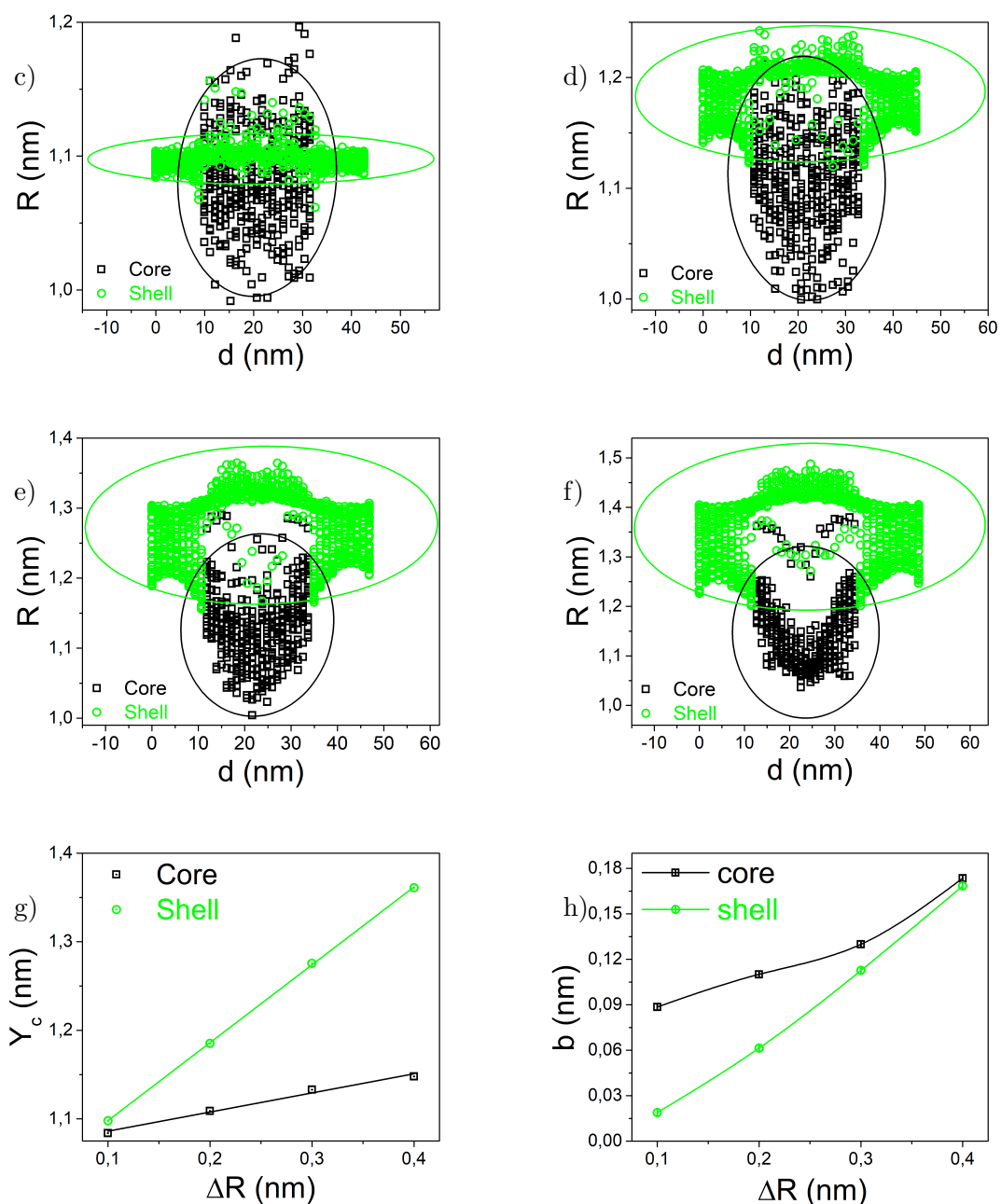


Fig. SM5: Quantitative density dependent position of intermolecular bond lengths,  $R$ , over a line crossing the nanoparticle as reported by the black arrow in the Fig. SM3 (a) for  $R_{shell} = 1.1$  nm (a), 1.2 nm (b), 1.3 nm (c) and 1.4 nm (d). (e) The Y coordinates of the ellipse center,  $Y_c$ , for the core (black) and the shell (green). (f) The semi-minor axis of the ellipse,  $b$ , for the core (black) and the shell (green).