Supplementary Material for

3D Elastic Modeling of Switchable Spin Transition Nanoparticles: Finite Size Scaling and Surface-bulk Interplay Effect on Thermal Hysteresis

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In this supplementary material we provide different movies and figures to shed light on the results already presented in the main manuscript by giving complementary information.

1 Movies

Movie S1 & S2: These videos show the spatiotemporal process of the electronic LS to HS (resp. HS to LS) phase transformation, including lattice deformations of the cubic nanoparticle of size $N = 64$, recorded during heating (resp. cooling) in video S1 (resp. S2) from $T = 50$ K (resp. $T = 130$ K) to $T = 130$ K (resp. $T = 50$ K). Yellow (blue) spheres represent HS (LS) sites. As the transition approaches, nucleation and growth of the new phase is observed to begin at the eight corners of the cube, followed by an isotropic propagation toward the center of the nanoparticle.

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2 Figures

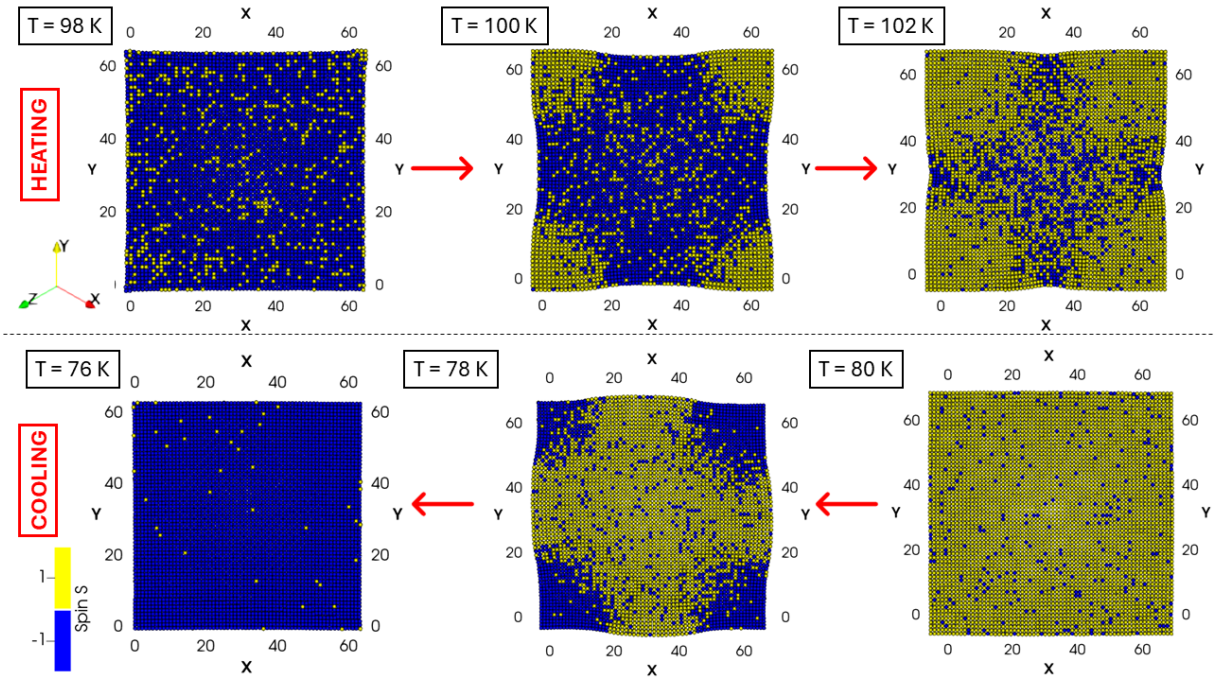

Figure S1 – Selection of snapshots illustrating 2D cross-sections perpendicular to the z-axis at an altitude of $z = \frac{3}{4}N$ ($N = 64$ is the nanoparticle size), during heating (top panels) and cooling (bottom panels), at various temperatures around the transition temperatures, $T_{up} \approx 101$ K and $T_{down} \approx 77$ K, corresponding to the 3D views of Fig. 2 of the main paper. Yellow (blue) spheres represent HS (LS) sites. In both cases, it is observed that during the HS-to-LS (and vice versa) transition, nucleation begins at the four corners of the squared sections, forming more or less circular interfaces, propagating isotropically toward the center of the nanoparticle.

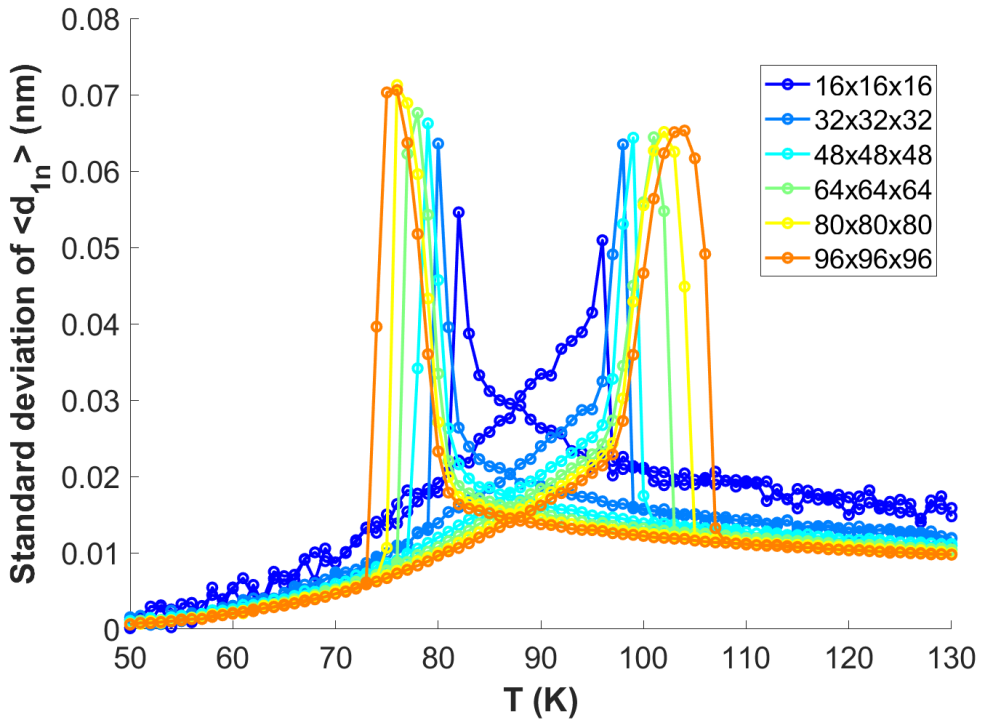

Figure S2 – Thermal dependence of error bars magnitudes of $\langle d_{1n} \rangle$, from Fig. 4 of the main paper, showing that they reach their maximum at the transition temperatures T_{up} and T_{down}, during heating and cooling, respectively.

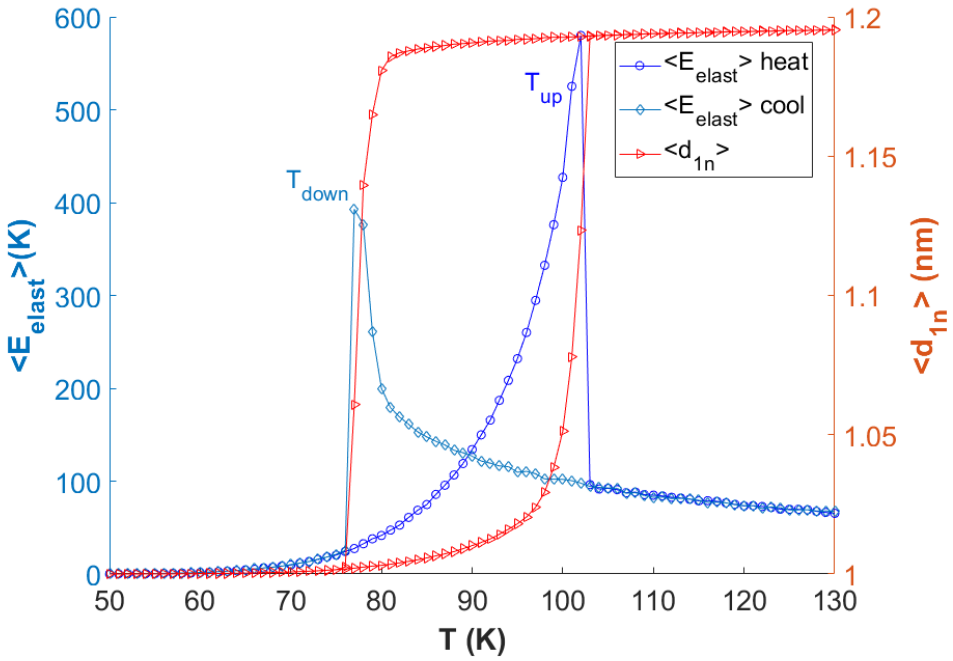

Figure S3 – Two-scale plot illustrating the thermal dependence of the average nearest-neighbor distance, $\langle d_{1n} \rangle$ (in red), alongside the thermal dependence of the total lattice elastic energy, $\langle E_{elast} \rangle$, for the heating and cooling branches of the hysteresis cycle for nanoparticle size $N = 64$ (in bluish). Transition temperatures T_{down} and T_{up} are marked to help the reader observe the close thermal correlation between $\langle d_{1n} \rangle$ and $\langle E_{elast} \rangle$. Identical trends were observed for other nanoparticle sizes previously discussed in the main manuscript.

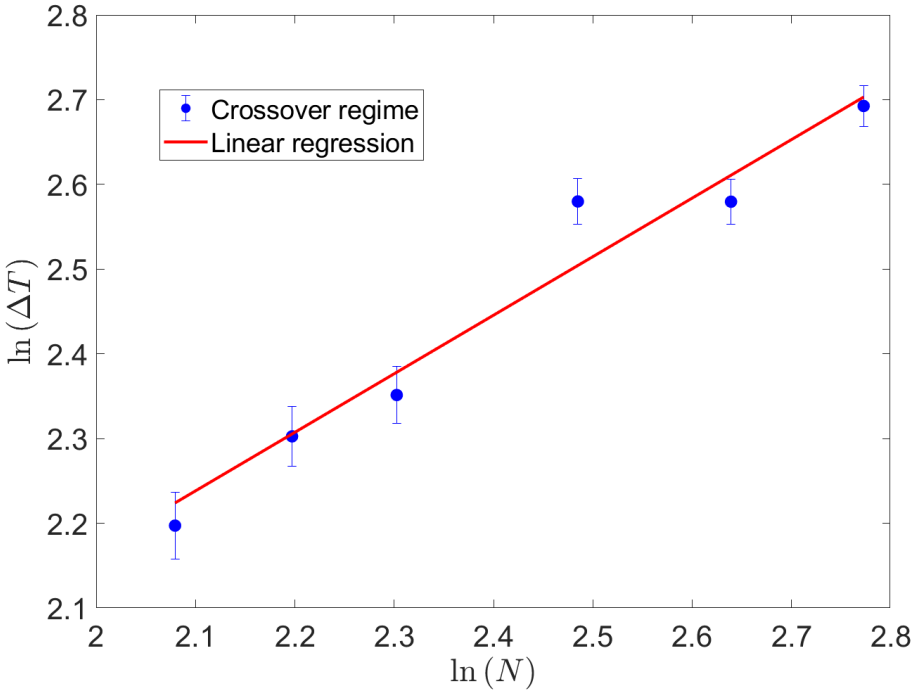

Figure S4 – Logarithm of the thermal hysteresis width, $\ln(\Delta T)$, vs $\ln(N)$, where N is the NP size, extracted from the points of the crossover regime of Fig. 5 of the main manuscript. The data are fitted with the linear regression (red dashed line) with a slope $\beta = 0.691 \pm 0.006$, indicating the existence of a power relation between ΔT and N. This behavior is phenomenologically analogous to that of a second-order phase transition, where ΔT plays the role of the order parameter and N that of the control parameter, which allows describing the bifurcation with the law $\Delta T \sim (N - N_{cri})^{\beta}$, where $N_{cri} \approx 6$ is the threshold size, and β is the corresponding effective exponent.

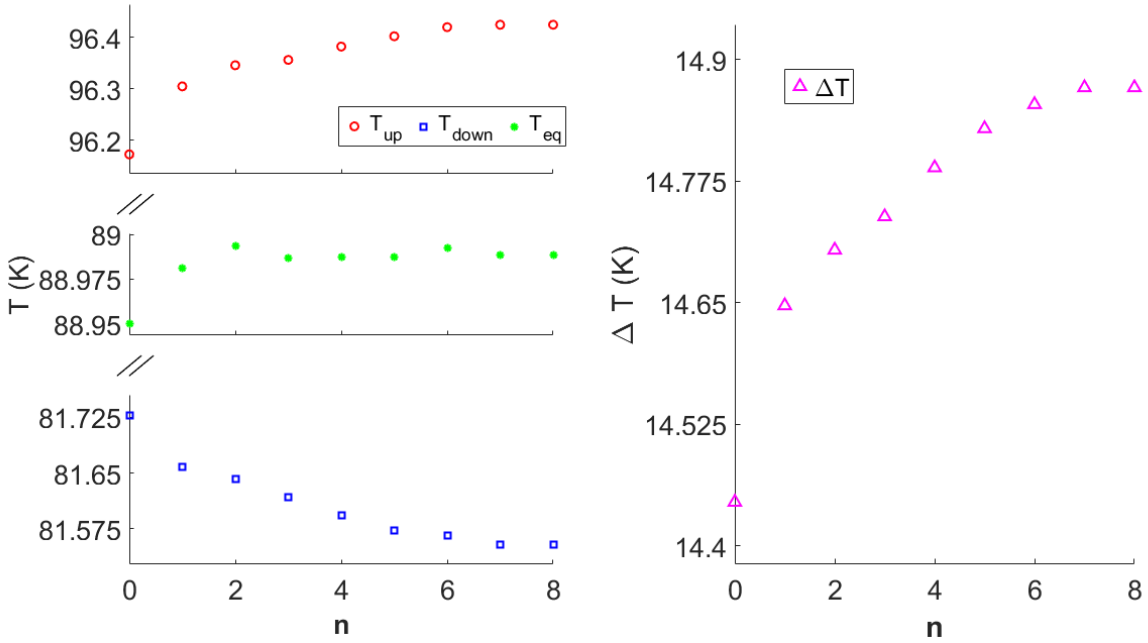

Figure S5 – Case of the nanoparticle with a small size $N = 16$. Left column: transition temperatures, measured on the surface of the concentric cubes, as a function of their distance n from the outer boundary of the 3D lattice, for the heating (T_{up}, red circles), cooling (T_{down}, blue squares), and for the equilibrium temperature ($T_{eq} = \frac{T_{up}+T_{down}}{2}$, green dots). A very slight deviation in transition temperatures is observed when moving from the edges of the nanoparticle toward its bulk. Right panel: hysteresis width $\Delta T = T_{up} - T_{down}$ as a function of n, showing a slight increase of the cooperative character for cubes that are as deep in the bulk as possible. Remark that a saturation is observed in the bulk in all cases.