Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The specific edge effects of 2D core/shell model for spin-crossover nanoparticles[1] AZUSA MURAOKA, Meiji University, KAMEL BOUKHEDDADEN, JORGE LINARÈS, FRANCOIS VARRET, Université de Versailles Saint-Quentin-en-Yvelines — We analyzed the size effect of spin-crossover nanoparticles at the edges of the 2D square lattices core/shell model, where the edge atoms are constrained to the high spin (HS) state. We performed MC simulations using the Ising-like Hamiltonian,

$$H = -J \sum_{(i,j)} \sum_{\substack{i' = \pm 1; \\ j' = \pm 1}} S(i,j)\, S(i+i', j+j') + \left(\frac{\Delta}{2} - \frac{k_B T}{2} \ln g \right) \sum_{(i,j)} S(i,j)$$

The molar entropy change is ΔS≈50J/K/mol, ln$g$ = ΔS/R≈6 (R is the perfect gas constant), energy gap is Δ=1300K. The HS fixed edges were based on the observation of an increasing residual HS fraction at low temperature upon particle size reduction. This specific boundary condition acts as a negative pressure which shifts downwards the equilibrium temperature. The interplay between the equilibrium temperature (=Δ/k$_B$ln$g$) variation and the expected variation of the effective interactions in the system leads to a non-monotonous dependence of the hysteresis loop width upon the particle size. We described how the occurrence condition of the first-order transition has to be adapted to the nanoscale.

[1]The present work has been supported by the Univ. Versailles, CNRS, GDRI France-Japan, and PRES-UniverSUd (COPECS project).

Azusa Muraoka
Meiji University

Date submitted: 07 Dec 2011 Electronic form version 1.4