STAGE de MASTER 2

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Ising-like model for 2D Spin Crossover nanoparticles: re-entrance phase transition"

Abstract

We will study the role of the interaction between edge molecules of the system with their local environment. We will use the Ising like model JLG taking into account short- long-range interaction (J and G respectively) and L, the environnement interaction. The Hamilton is:

$$H = \frac{\Delta}{2}\sum \sigma_i \; - J \sum_{\langle i,j \rangle} \sigma_i \, \sigma_j \; - G\langle\sigma\rangle \sum \sigma_i - \; L \sum_{k\; surface} \sigma_k$$

It can be written as:

$$H = \frac{\Delta - k_B T \; ln(g)}{2} \sum \sigma_i \; - J \sum_{\langle i,j \rangle} \sigma_i \, \sigma_j \; - G\langle\sigma\rangle \sum \sigma_i - \; L \sum_{k\; surface} \sigma_k$$

where g, in the rate between the degeneracy in the high-spin state (HS) and in the low-spin state (LS). In our preliminary results it has been found that by increasing the value of the edge interaction, L, the transition is shifted to the lower temperatures: it means that the role of edge interaction is equivalent to an applied negative pressure because the edge interaction favours the High-Spin (HS) state while the applied pressure favours the Low-Spin (LS) state.

The purpose of this work is to explain the re-entrance phase transition in nanoparticle SCO where the number of the molecules at the surface are bigger than in bulk.

References:

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2. D. Chiruta, J. Linares, P. Dahoo, M. Dimian, «Analysis of long-range interaction effects on phase transitions in two-step spin crossover chains by using Ising type systems and Monte Carlo entropic sampling technique", *Journal of Applied Physics, 12, 074906 (2012).*