Monte-Carlo simulations of the elastic frustration model and LIESST effect in spin crossover materials

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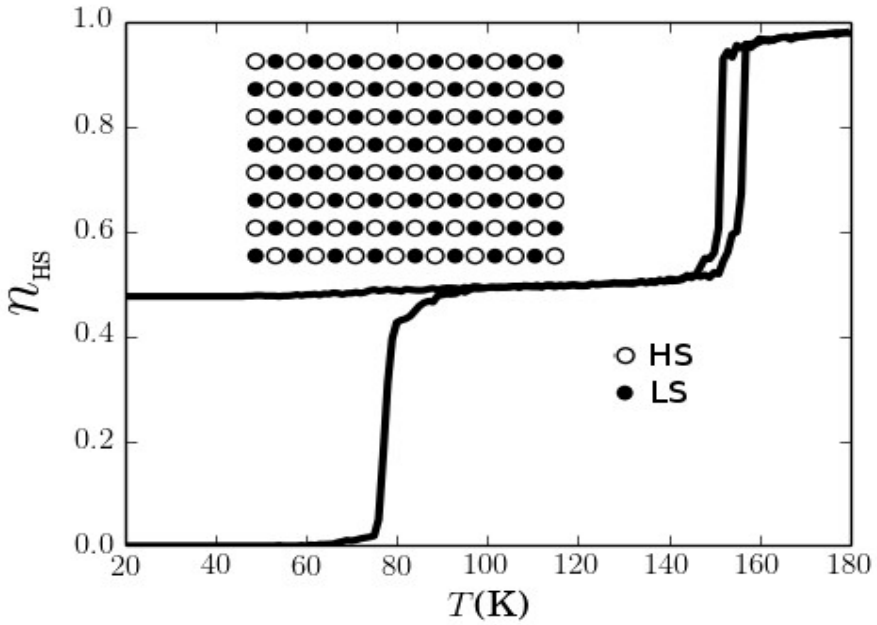
We have developed a microscopic electro-elastic model for spin crossover materials accounting for the volume change between high-spin (HS) and low-spin (LS) states using an harmonic potential for the elastic interaction. The competition between nearest neighbor (nn) and next nearest neighbor (nnn) equilibrium distances generates an elastic frustration which leads to a symmetry breaking. This model, fully elastic, let us obtaining first-order transition with hysteresis, gradual transformation, two-step, multi-step and incomplete transition with different patterns in the plateau regions [1].

We are going to compare the experimental results of the compound {Fe(2py-trz)[M(CN)4]} where M=Pt, Pd [2] which have an incomplete transition with the numerical simulation of the elastic model based on Monte-Carlo Metropolis method. This material also presents LIESST and reverse-LIESST effects and therefore we added this phenomena in the numerical resolution of the model in order to reproduce the complete behavior of the compound. We will show the spatial organization of the HS/LS fraction arising from the numerical results during the phase transition in temperature and under light.



[1] M. Paez-Espejo *et al.* JACS 2016, vol. 138 n. 9 pp 3202-3210
[2] E. Milin *et al.* Inorganic Chemistry 2016, vol. 55 n. 22 pp. 11652-11661