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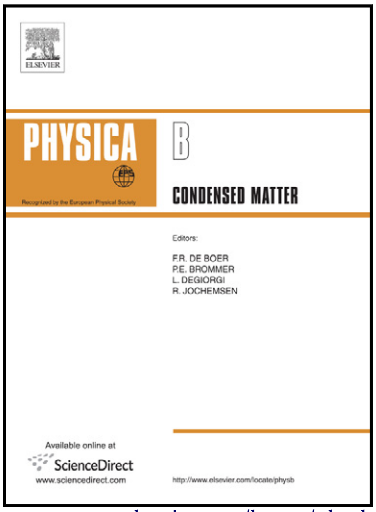

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Analysis of multi-step transitions in spin crossover nanochains

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Abstract The temperature driven phase transition occurring in spin crossover nanochains has been studied by an Ising-like model considering both short-range and long-range interactions. Various types of spin crossover profiles have been described in this framework, including a novel three-step transition identified in a nanosystem with eight molecules, which is modeled for the first time. A special interest has been also given to stepwise transitions accompanied by two hysteresis loops. The edge and size effects on spin crossover behavior have been investigated in order to get a deeper insight of the underlying mechanisms involved in these unusual spin transitions.

Keywords Ising model, short-range interaction, long-range interaction, multi-step transition

1. Introduction The last years have brought new research directions in the area of Fe^{II} spin crossover (SCO) complexes, one of these being the synthesis of switchable nanoparticles [1]. Investigating these materials at a reduced scale has attracted a significant interest due to their potential use in developing novel nanoelectronic and spintronic devices. In addition, their switching phenomena under a large range of stimuli (temperature, electrical field, pressure, magnetic field, light irradiation) [2-4] are of great importance and represent the focus of various research groups ranging from physics, chemistry, and material science communities [5-7]. To date, visualization [8] at reduced length scale is rapidly growing since the chemists have elaborated and applied synthetic methods for the production of nanoparticles embedded in a polymer matrix using e.g. reverse microemulsions [9-11], or trapped in silica thin films [12] of small dimensions (3-4 nm) [13]. Understanding the spin cooperation mechanisms and their influence on SCO processes is one of the main challenges in controlling these complex materials to design novel ones with specific properties. It is now widely accepted [14] that long range interactions between SCO molecules are of elastic origins and that depending on interaction strength, the SCO curve can display different shapes which can be gradual, abrupt, or in two-step with or without hysteresis [3]. The existence of hysteresis loops is intrinsically related to the spin cooperative phenomena, so it is of special interest for our current study.

Even if the understanding of the spin changing process from the LS to HS states or vice-versa require several experimental studies and a variety of models[15-19], the promising use of SCO materials in technical applications (i.e. recording devices, sensors, data storage, electroluminescent devices) [20] remain the principle motivation.

Two origins are given to explain the occurrence of two-step SCO transitions: i) an intrinsic structural inequivalence of two SCO sites [21] or ii) the existence of intermediate phases [22]. The LS-HS transition which results from the second origin provides an insight into the origin of short range