# Spin-crossover molecular hexagonal nanocrystal

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INTRODUCTION Spin-crossover complexes are transition metal coordination compounds that undergo reversible phase transitions between low-spin (LS) diamagnetic and high-spin (HS) paramagnetic states [1,2]. These materials have garnered significant interest due to their unique electronic bistability and potential applications. In this study, we investigate the spin-crossover transition in finite-sized hexagonal lattices (Fig.1), which serve as a realistic model for understanding spin-crossover behavior under experimental conditions. Our objective is to explore the influence of lattice geometry and intermolecular interactions on the occurrence of the spin-crossover transition in nanocrystals.

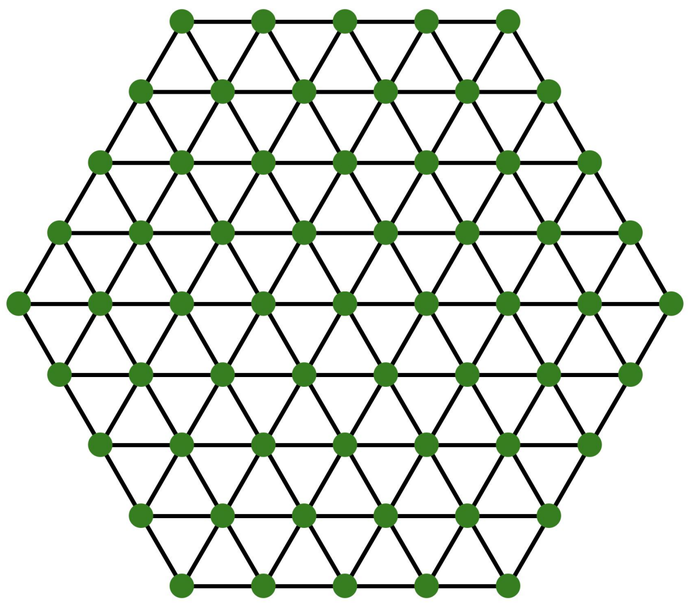


Fig. 1 An exemplary hexagonal (triangular) lattice comprising four layers, denoted as L4. In this configuration, each side of the lattice is encompassed by four rows of nodes, with a central node at the core.

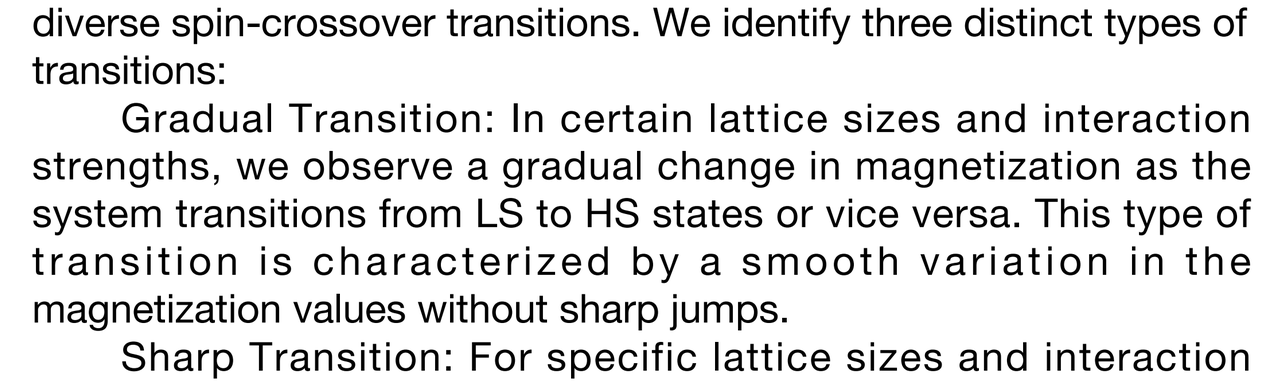
RESULTS Through Monte Carlo simulations using the Metropolis algorithm, we analyze the behavior of spin-crossover systems in hexagonal lattices of different sizes. By manipulating the lattice size and adjusting intermolecular interaction strengths, we calculate the system's magnetization and observe the emergence of diverse spin-crossover transitions. We identify three distinct types of transitions:

Gradual Transition: In certain lattice sizes and interaction strengths, we observe a gradual change in magnetization as the system transitions from LS to HS states or vice versa. This type of transition is characterized by a smooth variation in the magnetization values without sharp jumps.

Sharp Transition: For specific lattice sizes and interaction strengths, we observe sharp and sudden changes in magnetization, indicating a rapid transition between LS and HS states. These transitions exhibit well-defined critical points and are associated with pronounced changes in the system's properties.

Hysteresis Transition: In some cases, we observe hysteresis behavior, where the transition from LS to HS or vice versa occurs at different critical points depending on the direction of the transition. This hysteresis effect indicates the existence of metastable states and memory effects in the spin-crossover process.

All lattices in this study adhere to free boundary conditions, with L4 containing 61 sites (24 edge sites), L9 having 271 sites (54 edge sites), and L18 comprising 1027 sites (108 edge sites).



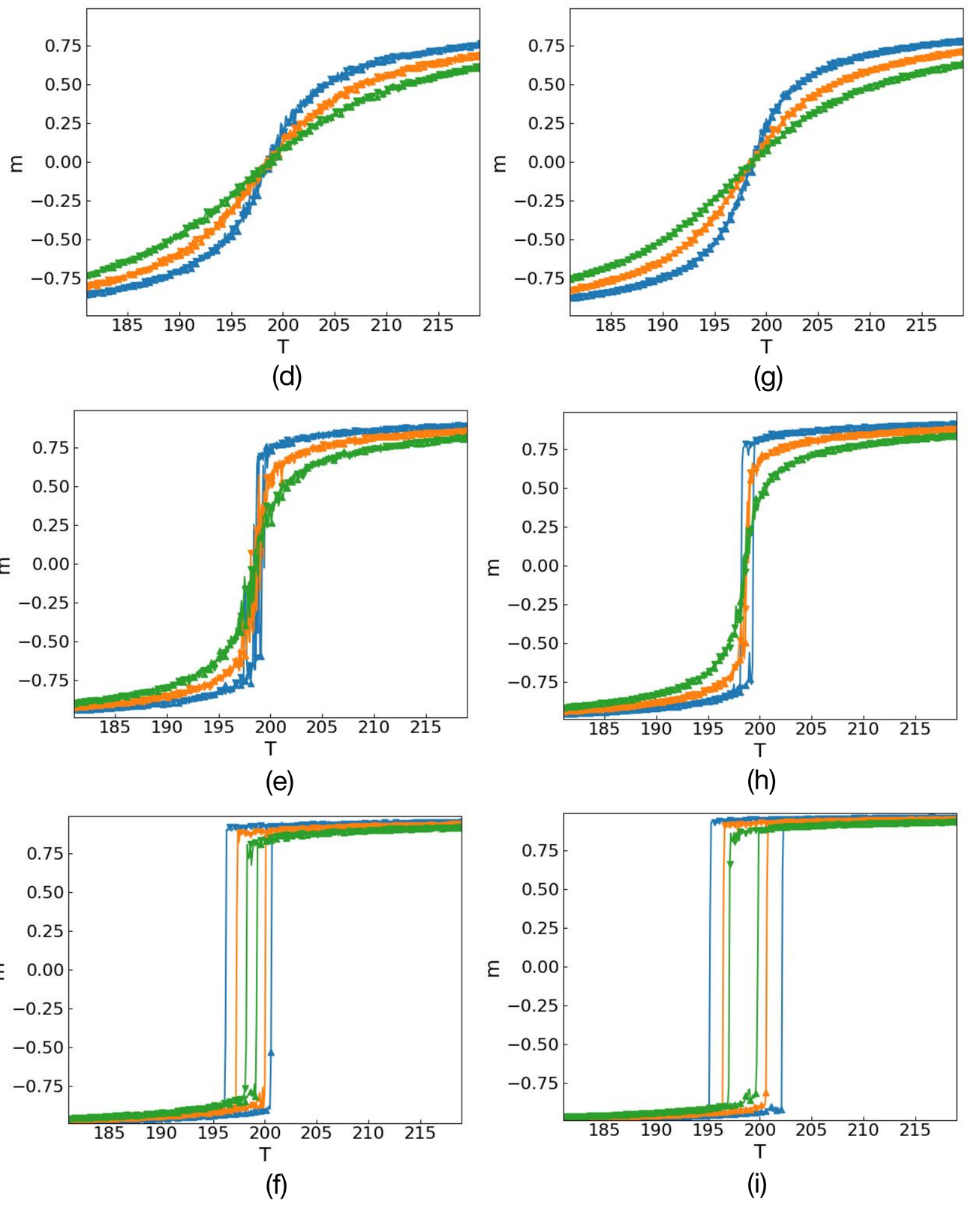




Fig. 2 Monte Carlo (MC) simulation results for magnetization < s > as a function of temperature. The figure comprises nine plots (a-i) representing gradual (a, d, g), sharp (b, e, h), and hysteresis (c, f, i) transitions. Each transition type is depicted for different lattice sizes: L4 (a-c), L9 (d-f), and L18 (g-i). The plots within each picture correspond to the following parameter values of J: gradual (J = 35, 40, 45), sharp (J = 50, 55, 60), hysteresis (J = 65, 70, 75) with green color marking the lowest J value and blue marking the highest. The other parameter values are Δ = 1000K and g = 150K.

The plots demonstrate (Fig. 2) the collapse of hysteresis with lower lattice sizes and sharper transitions with larger crystals. Additionally, the influence of lattice size on the smoothness of the results is evident.

SUMMARY

In summary, our Monte Carlo simulations in finite-sized hexagonal lattices provide insights into the nature of spin-crossover transitions in nanocrystals. We identify three types of transitions: gradual, sharp, and hysteresis. These different transition behaviors highlight the complex interplay between lattice geometry, intermolecular interactions, and the cooperative phenomena governing spin-crossover systems. Understanding these transition types is crucial for the design and optimization of spin-crossover materials with tailored properties for various applications.

REFERENCES

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