GROUND STATE OF KONDO-LATTICE MODEL FOR ORGANOMETALLIC FERROMAGNETS

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We have studied numerically the stability of the ferromagnetic ground state of organometallic ferromagnets such as the charge-transfer salt of decamethylferrocene and tetracyanoethylene described by the model Hamiltonian of a Kondo type. According to perturbation theory analyses, the increasing of the intra-atomic ferromagnetic exchange between d- and π-electrons leads to the destruction of the ferromagnetic ground state and to the appearance of the energy gap in the excitation spectrum of the lattice stack. The value of intra-atomic ferromagnetic exchange is sensitive to the changes of chemical structure of the organometallic ferromagnets. Therefore, the investigation of the model ground state spin as a function of electron parameters is of interest for a design of new magnetic materials. For the detail study of the stability of the ferromagnetic ground state the exact spectra of finite lattice clusters at different values of model parameters have been calculated. Considering the results of these calculations, we have shown that the transition between the states with marginal values of total spin is performed under the condition of local stability of ferromagnetic state against some spin-flops.

9.7 cm

13.4 cm

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