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Electron correlation effects in configurational model of doped fullerides

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Diversity of physical properties of doped fullerides has not been explained so far at a microscopic level despite the intensive experimental and theoretical studies conducted in recent decades [1]. The present study is devoted to investigation of electrical and magnetic properties interplay in the model [2] of a doped fulleride electronic subsystem with strong electron correlations, taking into account the orbital degeneracy, strong intra-atomic correlations and the correlated hopping of electrons. The importance of proper treatment for these interactions is caused by a competition between on-site Coulomb correlation (characterized by Hubbard parameter U) and delocalization processes (translational motion of electrons is determined by bare bandwidth and energy levels degeneracy). Energy spectrum of electronic subsystem and the ground state energy have been calculated within the Green function approach for configurational (in terms of Hubbard X-operators) representation [2, 3] of the model Hamiltonian. A generalization of the magnetization and Curie temperature calculations [4] has been developed which allows us to extend the phase diagram of the model and discuss driving forces for ferromagnetic state stabilization observed in Pt-doped fullerides [1]. The competition of itinerant behavior enhanced by the external pressure application and localization due to the correlation effects is discussed.

1. *Gunnarsson O.* Alkali-Doped Fullerides: Narrow-Band Solids with Unusual Properties. World Scientific Publishing Co., Singapore, 2004.
2. *Dovhopyaty Yu. et al.* Mott-Hubbard localization in a model of the electronic subsystem of doped fullerides // Ukr. J. Phys.- 2012.-**57**, N 9.-P. 920-928.
3. *Didukh L., Kramar O., Skorenkyy Yu.* Metallic ferromagnetism in a generalized Hubbard model / *in* New Developments in Ferromagnetism Research. Ed.: V.N. Murray.- Nova Science Publishers, Inc.- 2005.- pp. 39-80.
4. *Didukh L., Kramar O.* Metallic ferromagnetism in a generalized Hubbard model // Low Temp. Phys.-2002.- **28**, N 1.-P. 30-36.