Correlation effects in the model of orbitally degenerate electronic subsystem of fullerides: the configurational representation of Hamiltonian

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Despite the intensive experimental and theoretical studies, the diversity of physical properties of doped fullerides remains unexplained at a microscopic level. Doped systems A_3C_{60} (where A=K,Rb,Cs) turn out to be metallic at low temperatures. According to the theoretical band structure calculations (see [1] for review), fullerides with integer band-filling parameter n should be Mott-Hubbard insulators by electric nature, because all of them possess large enough values of intra-atomic Coulomb correlation parameter U. At the same time, in some of the doped fullerides (for example, AC_{60} and A_3C_{60}) a metallic state of unclear nature is realized. The present study is devoted to investigation of electrical and magnetic properties interplay in electronic subsystem of fullerides with strong electron correlations. In our study a model of doped fulleride electronic subsystem is formulated with taking into account the orbital degeneracy, strong intra-atomic correlations and the correlated hopping of electrons. The importance of proper accounting 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), which a realization of the insulating or metallic state depends on. Model Hamiltonian configurational representations for description of doped fullerides has been built. On a basis of the analysis carried out we argue that for an explanation of a metallic behavior of Mott-Hubbard system (x=3 corresponds to the half-filled conduction band) three-fold degeneracy of energy levels and Hund's rule coupling has to be properly taken into account. The possibility of metal-insulation transition in the system in the framework of the proposed model, is discussed.

1. Manini N., Tosatti E. E-print cond-mat/0602134.