Charge Ordering and Phase Separations In Itinerant Fermion Systems

W. R. Czart , P. Grzybowski and S. Robaszkiewicz

Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

We analyse the phase diagrams and thermodynamic properties of the charge orderings (CO) in narrow band materials using two effective models: (i) the spinless fermion model with repulsive intersite interaction ($W_{ij} > 0$) and (ii) the molecular crystal (MC) model with the coupling to intramolecular (crystal field) vibrations. We present results for the hypercubic lattices of infinite dimension ($d = \infty$) and compare them with the results for $d = 2$ square and $d = 3$ SC lattices. The calculations are performed within the (broken symmetry) HFA, which for the models with intersite interactions only, yield exact results for $d = \infty$. We focus our study on the problem of phase separations (PS) involving CO and the effects of next-nearest-neighbor hopping (t_2) on the charge ordered states in these systems. The ground state phase diagrams and the phase diagrams at finite temperatures are evaluated for several representative cases. The evolutions of basic characteristics of the systems in the CO states with the increasing interaction and a change of n are discussed. The results for $t_2 \neq 0$ are compared with those found for the case with nearest neighbor hopping only. The results we show here are an extension of our previous studies on the subject.