

Charge Orderings and Phase Separations In Itinerant Fermion Systems at Half Filling

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We analyse the ground state 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 case of half filled bands for the hypercubic lattices of infinite dimension ($d = \infty$) and compare them with the results for $d = 2$ square lattice. 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 are evaluated for several representative cases. 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.

← 13.4 cm →

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9.7 cm