The effects of the next-nearest neighbor density-density interaction in the atomic limit of the extended Hubbard model

Konrad Kapcia, Waldemar Kłobus, Stanisław Robaszkiewicz

Zakład Stanów Elektronowych Ciała Stałego, Wydział Fizyki,
Uniwersytet im Adama Mickiewicza, Umultowska 85, 61-614 Poznań,

A simple effective model of charge ordered insulators is studied. The tight binding Hamiltonian consists of the effective on-site interaction U and the intersite density-density interaction W_{ij} (both: nearest-neighbor and next-nearest-neighbor).

In the analysis of the phase diagrams and thermodynamic properties of this model we have adopted the variational approach, which treats the on-site interaction term exactly and the intersite interactions within the mean-field approximation. Within such an approach, only the particular cases have been studied till now. Moreover, the phase separated states have not been taken into account in those analysis.

Our investigation of the general case shows that, depending on the values of interaction parameters and the electron concentration, the system can exhibit not only homogeneous phases: charge ordered (CO) and nonordered (NO), but also various phase separated states (CO-NO, CO-CO). One shows that the systems considered can exhibit very interesting multicritical behaviors, including among others bicritical, tricritical, critical-end and isolated critical points..