GROUND-STATE PROPERTIES OF AN EXTENDED FALICOV-KIMBALL MODEL IN TWO DIMENSIONS

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A combination of the small cluster exact diagonalization technique and the own approximate numerical method has been used to study the ground-state properties of the two-dimensional Falicov-Kimball model extended by local interaction $U_{ff}$ between localized $f$ electrons. Phase diagrams, valence transitions as well as energy gaps have been calculated on finite clusters up to $L = 12 \times 12$ sites in the strong, intermediate and weak interaction limit of $U_{ff}$. In the strong and intermediate coupling limit ($U_{ff} > 2$) only the most homogeneous (insulating) and phase-separated (metallic) configurations are the ground states of the model. However, in the opposite limit ($U_{ff} \leq 2$) a new type of charge ordering corresponding to configurations with double occupied $f$ orbitals is formed. With decreasing $U_{ff}$ this metallic domain is further stabilized at the expense of the most homogeneous domain, while the phase separated domain remains practically unchanged. The meaning of these results for a description of real rare-earth materials is discussed.

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