

# 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.

13.4 cm

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9.7 cm