

GROUND-STATE PROPERTIES OF THE THREE-DIMENSIONAL FALICOV-KIMBALL MODEL

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The ground-state properties of the three-dimensional spinless Falicov-Kimball model are studied by a well-controlled numerical method. The results obtained are used to categorize the ground-state configurations according to common features for weak, intermediate and strong interactions. It is shown that only a few configuration types form the basic structure of the phase diagram. In particular, the largest regions of stability correspond to phase segregated configurations, striped configurations and configurations in which electrons are distributed in diagonal planes with incomplete chessboard structure. Near half-filling, mixtures of two phases with complete and incomplete chessboard structure are determined. In addition, the picture of valence and metal-insulator transitions is presented. The relevance of these results for a description of real material is discussed.

9.7 cm

13.4 cm

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