

substance: binary transition-metal oxides

property: considerations unique to transition-metal compounds

Three types of outer (outside closed atomic shells) electrons may be distinguished in solids: localized, itinerant with strong correlations, and itinerant with weak correlations. The former are adequately described by crystal-field theory supplemented, where interatomic interactions between like atoms are present, by magnetic superexchange or double-exchange theories. The latter are well described by conventional band theory. An adequate description of the intermediate case is more difficult; in general it requires the introduction of both strong correlations and strong electron-phonon coupling into the first-order band theory.

Conventional semiconductors contain only broad bands that are well described by normal band theory. Transition-metal compounds contain, in addition, narrow d bands; and the d electrons may be localized, itinerant with strong correlations, or itinerant with weak correlations. The physical properties they impart to the solid vary with both the population and character of the d electrons present. Therefore interpretation of the physical properties of transition-metal compounds depends upon two essential features: (1) placement of the d-state energies relative to the edges of the broad bands due to outer s and p electrons and (2) the character of the d electrons.