

COMMENTS ON THE MOTT-HUBBARD TRANSITION

J. B. Goodenough and J.-S. Zhou

Texas Materials Institute, ETC 9.102, The University of Texas at Austin
1 University Station, C2201, Austin, TX 78712

ABSTRACT

Comparison of the phase diagrams for the RMnO_3 and RNiO_3 families (R = rare-earth) show the influence of a strong intraatomic Hund exchange on the MnO_3 array, which approaches the Mott-Hubbard transition from the localized-electron side in LaMnO_3 , and of the stronger O-2p component in the e_g orbitals of the NiO_3 array, which passes through the Mott-Hubbard transition between SmNiO_3 and LaNiO_3 . The first-order character of the Mott-Hubbard transition at lower temperatures is demonstrated for mixed-valent as well as single-valent systems, for metal-metal as well as metal-oxygen-metal interactions. Comparisons of the transport properties of Fe_3O_4 above the Verwey transition with those of $\text{La}_{1-x}\text{Sr}_x\text{CuO}_4$, of the RMnO_3 family above the orbital-ordering temperature, and of the RNiO_3 family above the insulator-metal transition show that at higher temperatures the mobility of the charge carriers makes a smooth transition from polaronic to vibronic to itinerant behavior with increasing bandwidth.