

05.X-5 STRUCTURE AND PHYSICAL PROPERTIES OF SOLIDS. By John B. Goodenough, University of Oxford, Inorganic Chemistry Laboratory, South Parks Road, Oxford, OX1 3QR U.K.

The relationship between structure and physical properties is a fundamental theme in both science and technology. From the many topics of interest, the following are selected for review: (1) localized vs itinerant electrons, (2) spin states, (3) Jahn-Teller ordering vs charge-density waves, (4) mixed valency, (5) extended defects and dielectric anomalies, (6) ionic transport, (7) heterogeneous catalysis, and (8) influence of counter ions in mixed-metal systems.

05.X-7 MATERIALS WITH VALENCE INSTABILITIES. By E. Kaldis, Laboratorium für Festkörperphysik ETHZ, 8093 Zürich, Switzerland.

Valence instabilities appear in rare earth compounds (e.g. SmS, TmSe) with small 4f-5d energy gaps and NaCl structure. Hybridization of the strongly localized 4f states with the delocalized 5d states leads to valence fluctuations (homogeneously mixed valence). This phenomenon will be briefly discussed and the differences between mixed valence and the much more common mixture of valences will be stressed. With increasing 4f-5d gap the above hybridization is not any more possible and the tendency exists that the $4f^n$ and $4f^{n-1}$ states appear separately (coexist) in the crystal. An ideal structure to accommodate the separate but fluctuating valence states is the Th_3P_4 -structure ($\overline{1}\overline{4}3d-T_d^2$, $z=4$). This phenomenon will be briefly discussed in the examples of Eu_3S_4 and Sm_3S_4 . In this paper the possibilities to vary dramatically the physical properties through variation of structural and chemical parameters will be discussed. The thermodynamic properties of some of these systems will be presented with particular attention to valence induced thermodynamic phase instabilities.

05.X-6 On Properties of Solid State Metal Fluorides.

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Like corresponding oxides, Fluorides of metals are interesting materials for technical applications. For Solid State Fluorides a systematic search with respect to physical properties (e.g. magnetism, ferroelectricity, phase transitions, conductivity) seems successful only if conditions are valid which may be characterized by questions like:

A) How far implies a given composition in Solids what we call CHEMICAL CONSTITUTION?

B) Are those properties mentioned above strictly related to the chemical constitution only?

C) What sorts of systematic should we use for such fluorides with respect to this or that property wanted?

D) Is it possible to understand what we already know?

Typical examples shall illustrate possibilities, advances and limitations.

05.X-8 ANOMALOUS BEHAVIOUR OF PHYSICAL PROPERTIES AT PHASE TRANSITIONS. By A.M. Glazer, Clarendon Laboratory, Parks Rd., Oxford OX1 3PU, UK.

When a material undergoes a structural phase transition the atoms making up the crystal structure shift to new positions, often only through a very small distance. At the same time, many of the physical properties exhibited by the material change, often by surprising amounts. The reasons for such major changes and why they should be linked to very subtle movements of the constituent atoms are generally unknown, except in the case of a few special physical properties. By studying the structure by x-ray and neutron diffraction and the property of interest as a function of an external variable, typically temperature and pressure, it is often possible to establish which particular movements play an important role.

The results of such experiments will be described with application mainly to the so-called *ferroics*. The main properties to be discussed will be optical (birefringence, optical activity etc.) and electrical.