VALENCE INSTABILITY OF d-, f- ELEMENTS IN A CONFIGURATIONAL MODEL OF MATTER

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1. From the standpoint of the quantum field theory of electromagnetic matter the conceptual foundations Samsonov's configuration model of substance is discussed [1]. The main assumptions of this model and the ideological basis of the atomic and band models are compared within a single universal Hamiltonian of electron-nuclear system. It allows us to go beyond the standard scheme for self-consistent field and sort the main contributions of the nonlocal exchange-correlation interaction between electrons with different symmetry and different degree of localization. This opens the way to a consistent formulation of the dilemma "localization - collectivization" of the valence electrons. Embracing the extreme limits corresponding to the Hubbard model, Heisenberg, Ruderman-Kittel, Anderson, Kondo et al, our universal Hamiltonian provides the conceptual apparatus for correct quality interpolation between different limits [2]. .

2. The effects of the valence instability for the transition and rare earth elements in alloys and compounds are analyzed on the basis of quantum field theory. The concept of one-electron states (atomic shells, molecular orbitals, Bloch waves), successively filled "independent" electrons responsible only entry-level description of atoms, molecules or crystals. This is due to the replacement of the true particle interactions in the triad "particle-interaction-field" on the effective fields. Ignoring the effects of interparticle correlations does not allow to describe, for example, spontaneous rearrangement of the ground state in ferromagnets or superconductors, the appearance of elementary excitations of the polaron or exciton type, phase transitions of materials from dielectric to the metallic. .

3. Heuristic potency triad "composition-structure-property" in the theory of matter determined by the applicable concepts of normal valence in chemical elements and classic models of interatomic bonding. In materials containing transition and rare earth elements not only the structure but also its tendency to change under the influence of various external influences is a function of the composition. Source of general instability in this case may be instability of the structure of an isolated atom in acts of accepting, removing or excitation electron. Instability structure of d- and f-elements in the atomic state not only deprives these elements "legitimate" place in the Mendeleev's Periodic System, but also is the cause of irregular filling of their valence shell within large periods. For this reason, the material containing the d-and f-phase elements exist in a "zero", "amphoteric", "intermediate" and other abnormal values of valency, and their properties (depending on external conditions) detecting deviations from the ideal, regular or normal behavior of matter.

4. The foregoing provisions illustrated by the results of computer modeling of the thermodynamic, magnetic and electrical properties of the valence-unstable materials made using a variety of model Hamiltonians [3].

1. G.V.Samsonov, I.F.Pryadko, L.F.Pryadko. A Cofigurational Model of Matter.- N.Y.-L.: Consult. Bureau. - 1973.
2. Г.В.Самсонов, И.Ф.Прядко, Л.Ф.Прядко. Электронная локализация в твердом теле.- М.: Наука, 1976.
3. Л.Д.Дідух, Л.Ф.Прядко, І.В.Стасюк. Кореляційні эфекти в вузькозонних матеріалах. – Львів: Вища школа, 1978.