Metal-insulator transition in transition metal compounds: effect of orbital degeneracy and density of states peculiarities.

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For realistic theoretical description of electrical and magnetic properties of sulphides and selenides of transition metals, materials with strong electron correlations, one has to apply the orbitally degenerate Hubbard model [1,2]. It has been shown in papers [3,4] that the unperturbed density of states (DOS) form determines the critical concentration for occurrence of spontaneous ferromagnetic ordering. That justifies the necessity of approach [5] extension for a proper description of metal-insulator transition, forasmuch as DOS peculiarities affect directly the behavior of chemical potential and polar states concentration.

Using the variant [6] of generalized Hartree-Fock approximation in a limit of strong Coulomb correlation $U >> t$ and strong exchange interaction $U >> (U\text{-}J_H)$ in the present work the energy spectrum in a paramagnetic state at electron concentration $n = 1$ has been calculated. Transition from insulator to metallic state is accompanied by a closure of the energy gap

$$\Delta E = 3w\left(2d - \frac{1}{2}\right) + \frac{1}{2}\sqrt{\left[(U - J_H) + \frac{w}{2}\right]^2 + 32d^2w^2} + \frac{1}{2}\sqrt{\left[(U - J_H) - \frac{w}{2}\right]^2 + 32d^2w^2},$$

where $w = z|t|$ is halfwidth of energy band, U is energy of Coulomb repulsion of two electrons on different orbitals of the same site, J_H is energy of intra-atomic (Hund's rule) exchange, *d* stands for concentration of doubly occupied sites, determined by the DOS form. At fixed values of *U* and $t(\vec{k})$, i.e. constant external pressure and chemical composition, the dependence of *ΔE* on doublon concentration allows to study the metal-insulator transition under the external actions (temperature changes, magnetic field, etc) in transition metal compounds for which an orbital degeneracy of conduction bands is inherent. For example, the transition from metallic paramagnet state to Mott-Hubbard paramagnetic insulator state is realized in compounds NiS_2 and $NiS_{2-x}Se_x$.

On the basis of numerical calculations we have obtained the polar states concentration and energy gap width dependencies on energy parameters of the considered model and temperature for various model unperturbed DOS, in particular, semi-elliptic DOS, asymmetrical DOS with peak at the edge of energy band and DOS of simple cubic lattice. It has been found that DOS form slightly modifies concentration of doubly occupied sites and this effect is more pronounced for large on-site Coulomb interaction. In conclusion we note, that only at low temperatures the energy gap and metal-insulator transition in the considered model depend weakly on DOS form while at higher temperatures DOS form, determined by lattice symmetry, is decisive, especially for the case of asymmetrical DOS.

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