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Antisymmetric Exchange in Antiferromagnetic Materials of Rhombohedral Structures ALEXANDER BAZHAN, P.L.Kapitza Institute for Physical Problems, RAS, Moscow, Russia. — Carriers transferrings, determined by wave functions and energy levels of i j magnetic and oxygen ions, which are determined by rhombohedral oxygen crystal fields and their particularities, are in discussions for identification of antisymmetric, Dzyloshinskii-Moria exchange, $\mathbf{D}_z\{\mathbf{S}_{ix}\mathbf{S}_{jy}-\mathbf{S}_{iy}\mathbf{S}_{jx}\}$, taking into account Hubbard Hamiltonians, including spin-orbit interactions. Wave functions symmetry dependence are described by, depending on trigonal symmetry α, β coefficients in wave functions of energy levels of magnetic ions. Particularities of i j oxygen crystal fields are concerned with rotations of j fields at angles 60 degrees with respect to i fields. Taking spin-orbit, transferrings as perturbations, exchange symmetric,antisymmetric parts of spin Hamiltonians are $H_{ex} = \Sigma_{i,j}J_{i,j}(\mathbf{S}_i\cdot\mathbf{S}_j) + \Sigma_{i,j}\mathbf{D}_{i,j}[\mathbf{S}_i\times\mathbf{S}_j]$, where $J_{i,j}$ and $\mathbf{D}_{i,j}$ are determined by carriers transferrings, kinetic energies, Coulomb interactions, magnetic and oxygen energy levels. As examples, after some assumptions $\mathbf{D}_{ij}=$ $J\cdot(-\lambda)\cdot i\cdot\{\Sigma_m\langle\psi_{im}/\mathbf{L}_i/\psi_{i0}\rangle^*/(\varepsilon_{im}-\varepsilon_{i0})\cdot(t_{im,kn}/t_{i0,kn})$ - $\Sigma_m\langle\psi_{jm}/\mathbf{L}_j/\psi_{j0}\rangle^*/(\varepsilon_{jm}-\varepsilon_{j0})\cdot(t_{kn,jm}/t_{kn,j0})\}$, $\mathbf{D}_z \sim J\cdot\alpha\beta\cdot\{\lambda/(\varepsilon_m-\varepsilon_0)\}\cdot\{(t_{im,kn}/t_{i0,kn}-t_{kn,jm}/t_{kn,j0})\}$. Energy levels and Pauli requirements, determine depending on spin-orbit interactions, carriers transferrings between magnetic -oxygen -magnetic ions, which determine vectors $\mathbf{D}_z$, oriented, according to trigonal symmetry, along trigonal - z axis.

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