Multiband $d-p$ model and the electronic structure of doped quasi-two dimensional NiO_2 layer

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Superconductivity found in doped $NdNiO_2$ is puzzling as two local symmetries of doped NiO_2 layers compete [1], with presumably far-reaching implications for the involved superconductivity mechanism [1]. In spite of the great similarity between CuO_2 and NiO_2 planes, there are substantial differences in the electronic structure [2]. Along the family of infinite-layer nickelates RNiO$_2$ with rare-earth R spanning across the lanthanide series, the out-of-plane lattice constant decreases dramatically with an accompanying increase of Ni x^2-y^2 bandwidth; however, surprisingly, the role of oxygen charge transfer diminishes [3].

We introduce and investigate the multiband $d-p$ model (all d orbitals on Ni and p on O included), similarly to that used for $LaMnO_3$ compound [4], describing a quasi-two dimensional NiO_2 layer such as realized in $Nd_{1-x}Sr_xNiO_2$ [4] where superconductivity was discovered. The model takes into account anisotropic nickel-oxygen $d-p$ and oxygen-oxygen $p-p$ hopping processes, complicated crystal-field splittings, the on-site Coulomb repulsions and Hund's exchange tensors both at nickel and at oxygen ions. We investigate periodic boundary Ni$-$O clusters (4×4 and 8×8 NiO_2 units) with these interactions treated in the Hartree-Fock approximation [4]. The valence electron number n (per NiO_2 unit) is assumed to be approximately $n=21-x$ (due to surrounding Nd^{3+} and Sr^{2+} ions). Electronic structure of the layer is investigated for $x=0$, 0.125, 0.25 and 0.5. For ideal undoped system $NdNiO_2$ (no Sr admixture) we get strong insulator with degenerate ground state—both nonmagnetic, and magnetic (ferromagnetic, C-type and G-type antiferromagnetic) have all the same energy. However, for nonzero self-dopings x the system becomes conducting (zero HOMO-LUMO gap), also with quasi-degenerate ground state due to numerous competing magnetic metastable states. (Possibilities of getting locally triplet states at Ni ions are also investigated, similarly as in [5]). These findings correlate well with experimental data and with other theoretical predictions available in the literature.

References:

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