MODELLING CHARGE, ORBITAL AND MAGNETIC ORDER IN $La_{1-x}Sr_xMnO_4$ MONOLAYER MANGANITES

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The model which describes correlated e_g electrons in doped, monolayer manganites [1] was recently studied by using correlated wave functions [2]. The effective Hamiltonian [3] takes into account: the kinetic energy of e_g electrons, the crystal-field splitting between $x^2 - y^2$ and $3z^2 - r^2$ orbitals, on-site Coulomb interactions, the interaction between e_g electrons and core S = 3/2 spins due to t_{2g} electrons, antiferromagnetic superexchange interaction between core spins, and finally the coupling between e_g electrons and Jahn-Teller modes. We have demonstrated that this model is in general capable of reproducing the phase situation in monolayer manganites [3]. Quite recently, it was found [4] that the splitting between the occupied and empty e_g states at every site is quite large in $La_{1-x}Sr_xMnO_4$ (exceeding by far any previous estimates) and here we investigate the reasons and physical consequences of this large splitting.

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Subject category :

1. Strongly Correlated Electrons and High Temperature Superconductivity

Presentation mode : poster

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 $9.7~\mathrm{cm}$