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LaNiO3/LaAlO3 heterostructures: A LDA+DMFT analysis

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The discovery of high temperature superconductivity in cuprates [1] initiated the quest for finding related transition metal oxides with comparable or even higher transition temperatures. The family of nickel oxides have been subject to investigation for some time in order to find similarities and differences to isoelectronic cuprate structures [2]. The emerging possibilities to synthesize transition metal oxide heterostructures open new opportunities in this respect. We investigate the $LaNiO_3/LaAlO_3$ heterostructure [3]. In the threevalent Ni^{3+} the two Nickel e_g states $|x^2-y^2\rangle$ and $|3z^2-r^2\rangle$ are occupied by one electron. Our analysis was performed with the local density approximation (LDA) and its combination with dynamical mean field theory (LDA+DMFT)[4]. The quasi 2D-character of the system may suggest, that the $|3z^2-r^2\rangle$ states – which barely overlap in the xy-plane – play only a negligible role. However, this is not true since the hopping processes from the $|3z^2-r^2\rangle$ to the highly mobile $|x^2-y^2\rangle$ states are by no means small. In this way additional mobility is given to the $|3z^2-r^2\rangle$ states, which enriches the physical features of the system.
The interaction effects in the Nickel e_g states were treated within a two band model at quarter filling. The effective Hamiltonian for this system reads

$$\hat{H}_{eff.} = \sum_{iljm,\sigma} t_{iljm} c^{\dagger}_{il\sigma} c_{jm\sigma} + U \sum_{il\sigma} n^{\sigma}_{il} n^{-\sigma}_{il} + \sum_{il \neq m\sigma\sigma'} (V - \delta_{\sigma,\sigma'} J) n^{\sigma}_{il} n^{\sigma'}_{im} \,, \qquad (1)$$

where $c_{il\sigma}$ ($c^{\dagger}_{il\sigma}$) annihilates (creates) an electron on Ni site i, in orbital l with spin σ, $n^{\sigma}_{il} = c^{\dagger}_{il\sigma} c_{il\sigma}$, $\delta_{\sigma,\sigma'}$ denotes the Kronecker symbol, U and V represent the intra-orbital and inter-orbital repulsion respectively and J is the Hund exchange term. Hamiltonian (1) was then solved by means of the DMFT using a Hirsh Fye Quantum Monte Calro impurity solver. The results for the paramagnetic/high-temperature phase show that both bands remain metallic and contribute to the Fermi surface, unless the Coulomb interaction is turned to unrealistically large values. For investigating possible ordering tendencies at low temperatures the exchange parameters of an effective Kugel-Khomskii-like spin-orbital-model [5] were derived within an effective two site calculation. The results indicate the presence of strong antiferromagnetic fluctuations which might drive the heterostructure on the insulating side of the metal insulator transition at low temperatures. Such antiferromagnetic fluctuations are also considered to be essential for high temperature superconductivity.

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