Abstract Submitted
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Competition between ferromagnetism and superconductivity in hole and electron doped cuprates B. BARBIELLINI, Northeastern U., T. JARLBORG, University of Geneva, H. LIN, R. S. MARKIEWICZ, A. BANSIL, Northeastern U. — Band calculations for supercells of $La_{2-x}Ba_xCuO_4$ beyond the rigid band model give support to the idea that weak ferromagnetism can be the cause of the destruction of superconductivity at high hole doping [1,2]. We are exploring similar mechanisms in the electron doped $Nd_{2-x}Ce_xCuO_4$. In this case, the treatment of the Nd and Ce f electrons presents new challenges. For this reason, we compare spin-polarized DFT results which include the Nd-f (and Ce-f) electron in the valence band with calculations in which the Nd-f electrons are forced to be core states. Our simulations use both the simple unit cell and $2 \times 2 \times 1$ supercells in various magnetic configurations (i.e. ferromagnetic, antiferromagnetic and ferrimagnetic). The results indicate that subtle charge transfers and screening occuring near the Ce impurity may give interesting Coulombic effects between the Nd/Ce and CuO planes [3]. Work supported in part by the US DOE.
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