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Density-functional theory calculation of Fermi surface in stripe ordered $YBa_2Cu_3O_{6.5}$ SIMON BLACKBURN, MICHEL COTE, University of Montreal — High temperature superconductors (HTSC) attract a lot of interests since their discovery in 1986. More recently, observations of quantum oscillations in underdoped $YBa_2Cu_3O_{6.5}$ (YBCO6.5) at a low frequency suggested a small pocket constitute the Fermi surface (Doiron-Leyraud et al. Nature 447, 565 (2007)). In this work, we present results of density-functional theory (DFT) calculations of YBCO electronic structure. In order to better represent the electron-electron interaction, we add an on-site repulsion term (Hubbard term) on the copper d-orbitals (DFT+U). This method is known to improve DFT calculations for Mott insulators like La_2CuO_4 and $YBCO_{6.0}$ since the Hubbard term favors an anti-ferromagnetic ground state. Using this method, we compare various magnetic states calculated with different values of the Hubbard term U. Our results suggest that an atom-centered stripe, similar to the one found in $La_{1.875}Sr_{0.125}CuO4$ (Tranquada et al. Nature 375 561 (1995)), is consistent with the presence of a Fermi pocket of the size reported in the experiments. We further show that the size of the pocket and the nature of the carriers (electrons or holes) can be varied with pressure suggesting a way to test this hypothesis.

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