

Electronic Structure of Striped Phase of $\text{Ca}_{1.875}\text{Na}_{0.125}\text{CuO}_2\text{Cl}_2$

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Charge and spin-density waves known as stripes have been observed in a number of cuprates and are usually best observed at a hole concentration of $1/8$ per copper ion. They have been imaged in real space using scanning tunnelling conductance measurements [1,2] and spin waves associated with them have been observed by neutron scattering [3,4]. We present hybrid density functional theory calculations on unidirectional and intersecting magnetic anti-phase boundaries (APB) in $\text{Ca}_{1.875}\text{Na}_{0.125}\text{CuO}_2\text{Cl}_2$. We show that APB consist of parallel arrays of Emery-Reiter spin polarons [5] and that these may explain the observed stripe state in $1/8$ doped cuprates in terms of polaronic oxygen ions which induce ferromagnetic coupling of neighboring copper ions. Since spins on neighboring copper ions in the stripe are parallel, the stripe forms an APB between anti-ferromagnetically ordered regions of copper spins separated by four lattice constants. We also consider an ordered spin polaron phase where magnetic anti-phase boundaries intersect at right angles. In this case, sets of four copper ions in squares at stripe intersections have parallel spins. This phase may be the 4×4 checkerboard pattern reported by Hanaguri *et al.* [1]. Hybrid density functional calculations on small polarons in $\text{Ca}_{1.97}\text{Na}_{0.03}\text{CuO}_2\text{Cl}_2$ show that they are localized on clusters of five copper ions and have ferromagnetically coupled spins. They have strong repulsive interactions and induce localized virtual states in the band gap.

[1] T. Hanaguri *et al.* Nature **430**, 1001 (2004).

[2] Y. Kohsaka *et al.* Science **315**, 1380 (2007).

[3] S. M. Hayden *et al.* Nature **429**, 531 (2004).

[4] J. M. Tranquada *et al.* Nature **429**, 534 (2004).

[5] V. J. Emery and G. Reiter, Phys. Rev. B **38**, 4547 (1988).