Visualizing the atomic and molecular orbital basis for pair formation in cuprate

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The parent compound of cuprate high temperature superconductors is a charge-transfer-type Mott insulator with strong hybridization between the Cu $3d_{x2-y2}$ and O $2p$ orbitals. A key question concerning the pairing mechanism is the behavior of doped holes in the antiferromagnetic (AF) Mott insulator background, which is a prototypical quantum many-body problem. Scanning tunneling microscopy (STM) represents an ideal experimental technique to address these questions owing to its capability of atomic-scale imaging of local electronic states.

In this work, we use STM to visualize the electronic structure of diluted holes doped into the $Ca_2CuO_2Cl_2$ parent Mott insulator of cuprates. We find that a single hole exhibits an in-gap electronic state and clover-shaped spatial distribution reminiscent of an extended d_{x2-y2} atomic orbital. For multiple dopants lying in close proximity, the overlap of wavefunctions generates stripe- and ladder-shaped molecular orbitals, accompanied by the opening of a precursory energy gap around the Fermi level. With increasing doping, the molecular patterns proliferate in space and gradually form densely packed plaquettes with characteristic length scale around 4 a_0. A full-fledged superconducting gap develops smoothly on top of the molecular orbitals, and display a systematic evolution of gap function. These results demonstrate that the stripe-like molecular orbital is the first low energy electronic state induced by doping the antiferromagnetic Mott insulator, and a local Cooper pair is formed by two holes occupying a molecular plaquette.

References:

1. Shusen Ye et al., *Nature Physics* 19, 1301 (2023)
2. Shusen Ye et al., arXiv: 2309.09260 (2023)