Sci. Bull.
DOI 10.1007/s11434-016-1204-x

www.scibull.com
www.springer.com/scp

Article

Physics & Astronomy

Relationship between the parent charge transfer gap and maximum transition temperature in cuprates

Wei Ruan · Cheng Hu · Jianfa Zhao · Peng Cai · Yingying Peng · Cun Ye · Runze Yu · Xintong Li · Zhenqi Hao · Changqing Jin · Xingjiang Zhou · Zheng-Yu Weng · Yayu Wang

Received: 3 November 2016 / Revised: 8 November 2016 / Accepted: 9 November 2016

Abstract One of the biggest puzzles concerning the cuprate high temperature superconductors is what determines the maximum transition temperature ($T_{c,max}$), which varies from less than 30 to above 130 K in different compounds. Despite this dramatic variation, a robust trend is that within each family, the double-layer compound always has higher $T_{c,max}$ than the single-layer counterpart. Here we use scanning tunneling microscopy to investigate the electronic structure of four cuprate parent compounds belonging to two different families. We find that within each family, the double layer compound has a much smaller charge transfer gap size (Δ_{CT}), indicating a clear anticorrelation between Δ_{CT} and $T_{c,max}$. These results suggest that the charge transfer gap plays a key role in the superconducting physics of cuprates, which shed important new light on the high T_c mechanism from doped Mott insulator perspective.

W. Ruan · P. Cai · C. Ye · X. Li · Z. Hao · Y. Wang (✉)
State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China
e-mail: yayuwang@tsinghua.edu.cn

C. Hu · J. Zhao · Y. Peng · R. Yu · C. Jin · X. Zhou
Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

C. Jin · X. Zhou · Z.-Y. Weng · Y. Wang
Collaborative Innovation Center of Quantum Matter, Beijing 100084, China

Z.-Y. Weng
Institute for Advanced Study, Tsinghua University, Beijing 100084, China

Keywords Cuprates · Mott insulator · Charge transfer gap · Maximum transition temperature · Scanning tunneling microscopy

1 Introduction

Since the discovery of copper oxide (cuprate) high temperature superconductors about 30 years ago, understanding its microscopic origin has become one of the greatest challenges in condensed matter physics. The problem is well-defined, i.e., to find the mechanism of Cooper pairing for charge carriers residing in the two-dimensional CuO_2 plane that is common to all cuprates. However, after decades of experimental and theoretical investigations, very few consensuses have been reached [1–5]. Figure 1a displays the schematic phase diagram of hole-doped cuprates, in which only two well-defined phases are unambiguously determined. First, the parent compound is an antiferromagnetic (AF) Mott insulator due to strong onsite Coulomb repulsion, and the long-range AF order is suppressed by hole doping. Second, the superconducting (SC) phase exists in a range of hole concentrations, and the $T_{c,max}$ is reached at optimal doping near the center of the dome. The definition and doping dependence of other phases, such as the pseudogap phase [6] and charge orders in the underdoped regime [5], are still under much debate.

One of the central issues about the cuprates is what determines the $T_{c,max}$ of a specific system, which varies dramatically from 25 to 138 K in ambient pressure [7]. A highly robust, but yet mysterious trend is that within each family the double-layer compound has much higher $T_{c,max}$ than the single-layer counterpart. Finding the physical parameter that controls $T_{c,max}$ is apparently a key step for solving the high T_c superconductivity puzzle. For

Published online: 23 November 2016

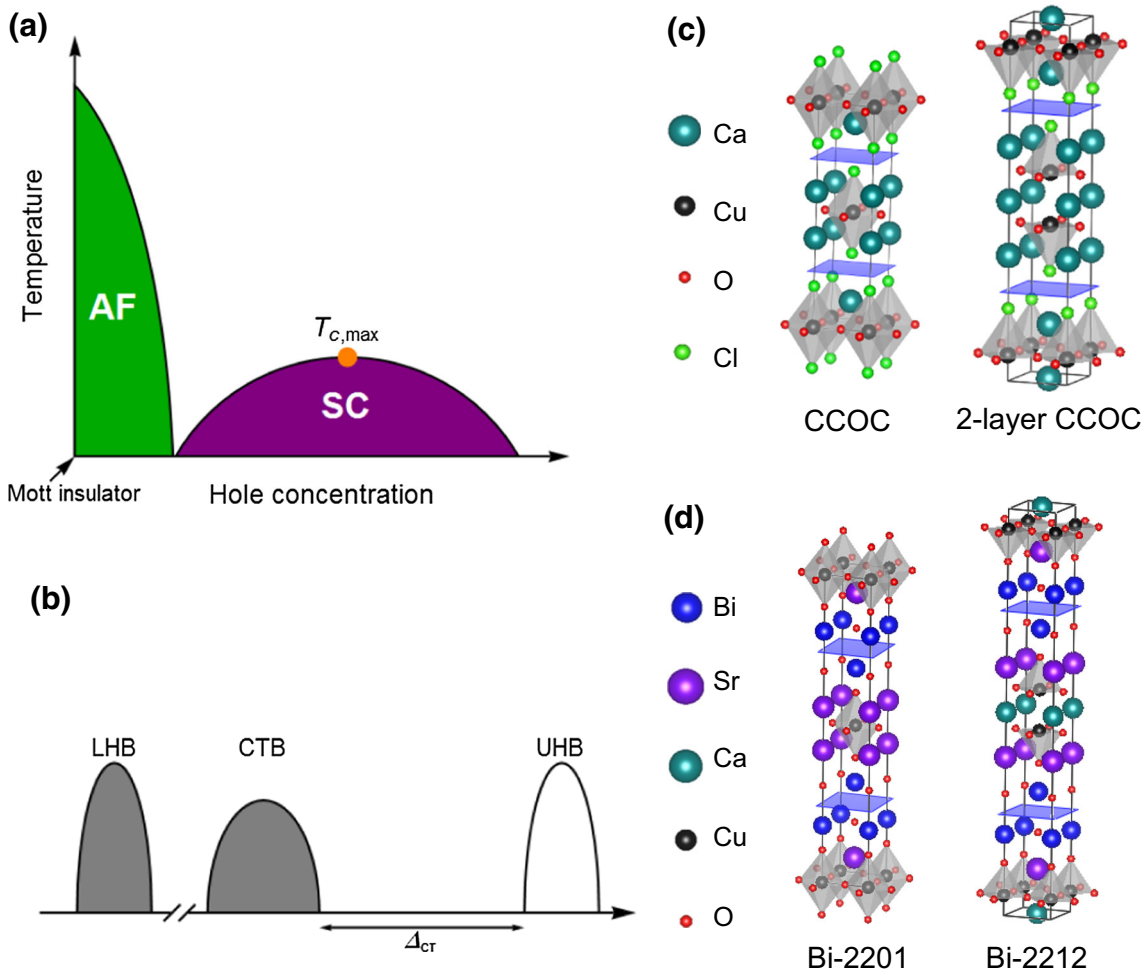

Fig. 1 (Color online) Phase diagram of hole-doped cuprates and crystal structure of the four materials studied here. **a** Schematic electronic phase diagram of hole-doped cuprates, showing the parent Mott insulator, the AF phase and the SC dome. The maximum SC transition temperature is marked by the orange dot. **b** Schematic band structure of parent cuprate. The charge transfer gap Δ_{CT} is the energy distance between the UHB and the CTB. **c** The crystal structure of $Ca_2CuO_2Cl_2$ (CCOC) and $Ca_3Cu_2O_4Cl_2$ (2-layer CCOC), respectively. **d** The crystal structure of $Bi_2(Sr,La)_2CuO_{6+\delta}$ (Bi-2201) and $Bi_2Sr_2(Ca,Dy)Cu_2O_{8+\delta}$ (Bi-2212), respectively

conventional BCS (Bardeen-Cooper-Schrieffer) superconductors, for example, a crucial breakthrough for the final resolution of phonon-mediated mechanism is the discovery of the isotope effect $T_c \sim m^{-1/2}$, where m is the isotopic mass [8, 9]. For the cuprates, there were previous attempts to find the scaling relation between T_c and other physical parameters, such as superfluid density [10] and metallic conductivity near T_c [11]. However, these are macroscopic properties of the SC phase itself, which dictate the phase transition phenomenology but provide little hint regarding the origin of Cooper pairing in the first place. It is highly desirable to find a direct connection between $T_{c,max}$ and the microscopic electronic structure, especially that of the parent compound from where superconductivity emerges.

The most relevant bands of the cuprates derive from the Cu $3d_{x^2-y^2}$ orbital and two O $2p$ orbitals in the CuO_2 plane [12], as schematically drawn in Fig. 1b. Due to strong onsite Coulomb repulsion and relatively small charge transfer energy, the half-filled parent compound is a Mott insulator of the charge transfer type [13]. The hopping integral between O and Cu sites, as well as the onsite and off-site Coulomb repulsions, may all affect the behavior of doped charges hence $T_{c,max}$. Despite this complexity, we notice that the most significant energy scale in the electronic structure of parent cuprate is the charge transfer gap (CTG) between the upper Hubbard band (UHB) and the charge transfer band (CTB, or the Zhang-Rice singlet band), which characterizes the energy needed for an O site electron to migrate to the neighboring Cu sites [14]. If the doped Mott insulator picture is indeed the valid theory for high T_c superconductivity, there might exist a direct link between the CTG size Δ_{CT} in the parent compound and $T_{c,max}$ at the optimal doping. In a recent theoretical work, the charge transfer energy ε_d–ε_p of various cuprates was