# Cluster Orbital for Granular Superconductivity of Underdoped Bi2212

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**Abstract**

A model of the inhomogeneously doped lattice for Bi-2212 is presented based on the structure of infinite layer cuprates. The ab initio molecular orbital (MO) calculation on the model cluster, $Cu_{24}O_{50}Ca_6Sr_{15}$ , showed that the coupling of $Cu3d_{x^2-y^2}$ and O $2p\pi$ orbitals is important in the highest occupied MO (HOMO) which might be mediated through the coupling of s orbitals of alkaline earth ions on the outer layers with the orbitals of the $CuO_2$ plane. A new aspect of coupling force in the Cooper pair is present.

*Key words:* superconductivity mechanism; cluster orbital; Cooper pair

## 1. Introduction

The origin of attractive force in the Cooper pair of cuprates is a challenging problem of physics and chemistry of superconductivity (SC). Recently Davis et al [1] found a granular SC in the underdoped (14 %) and optimally doped (18 %) Bi-2212 and showed that the superconducting gap is higher in the domain as small as 1.3 *nm* radius. We have continued ab initio molecular orbital calculation of the model clusters of cuprates to find the orbitals responsible for metallic and SC states. [2] The doping induced insulator to metal transition is reasonably explained on one-dimensional chain, in which models are made referring the infinite layer crystal. [3] The vacancies $x$ of alkaline earth ion layer in $(Ca,Sr)_{1-x}CuO_2$ gives exactly the same effect $x$ in $La_{2-x}(Ba/Sr)_xCuO_4$. The doping dependence of SC has been studied most extensively on $La_{2-x}(Ba/Sr)_xCuO_4$ and it is established that $x = 0.14$ is in the region of optimum doping. The gap map of 14 % doped Bi-2212 clarified [1] the structure of inhomogeneously doped lattice. In this paper we propose the model of 14% doped lattice in which the high and low dopants regions coexist. The cluster orbital for the high concentration domain is calculated to find the relevant HOMO for Cooper pair formation.

## 2. Result

In Fig.1 the model for 14 % doped lattice is illustrated, where the small black dots show copper ion on the $CuO_2$ plane and small white circles are the position of the vacancies in the alkaline earth ion layer. The large circles with 1.3 *nm* radius includes about 32 Cu ions and 64 O ions. The high gap energy ($\Delta$) domain is supposed to be within the circle where the dopant concentration is higher than in other region. Outside of these circles, the dopant concentration is low, but they are enough for maintenance of metallic state.[2] By increasing the dopant, the low dopant region is narrowed, and at 25 % doping the whole lattice is homogeneously covered with dopants arranged by the same pattern within the circle of Fig.1.

We performed molecular orbital calculation by uB3LYP method of Gaussian 98 programs on model clusters, and found the most stable UHF solution; the $\alpha$-spin HOMO (A) and the $\beta$-spin HOMO (B) of

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$Cu_{24}O_{50}Ca_6Sr_{15}$ are as shown in Fig.2. In this figure small black dots are Cu sites and white circles are vacancies of alkaline earth ions. The + and − signs on the left column illustrates the + and − signs of $Cu3d_{x^2-y^2}$ orbitals as shown on the top left. The rectangular boxes are abbreviation for the group of O2p$\pi$ orbitals, which shape is illustrated on the top right. Four boxes in the right column (B) are related by a $D_{4h}$ symmetry. The $\alpha$-spin orbital (A) contains also some O 2p$\pi$ orbitals . These MOs are obtained by a configuration interaction of the next HOMO and the LUMO of RHF calculation. The next HOMO is composed of mostly $Cu3d_{x^2-y^2}$ and the LUMO is comprised of mostly O2p$\pi$ orbitals and both of them contain some 3s and 4s orbitals of Ca or Sr in the alkaline earth ion layer with the same shape and symmetry. The symmetries of $Cu3d_{x^2-y^2}$ and O2p$\pi$ are different and they could not couple directly, but the associated Ca and Sr orbitals in the next HOMO and LUMO have exactly the same shape and symmetry. As a result of the configuration interaction of these orbitals they are mixed to give a UHF solution which gives most stabilized state compared to the other solutions. The resultant MOs have different shape as shown in Fig.2. Accordingly the attractive energy between the $\alpha$-spin HOMO (A) and $\beta$-spin HOMO (B) is attributed to the coupling of O2p$\pi$ orbitals in (A) and (B) and the interaction through the outer layer s orbitals. The alkaline earth orbitals mediate the coupling of $Cu3d_{x^2-y^2}$ and O2p$\pi$ in properly doped cuprates.

Two aspects of Cooper pair in cuprates are apparent; one is the coupling of different shaped $\alpha$-spin (A) and $\beta$-spin (B) orbitals, and another is a source of attractive force via the s orbitals of the outer layer. To explore the real space images and interactions is important for future studies of high Tc SC from both chemical and physicical points of view.

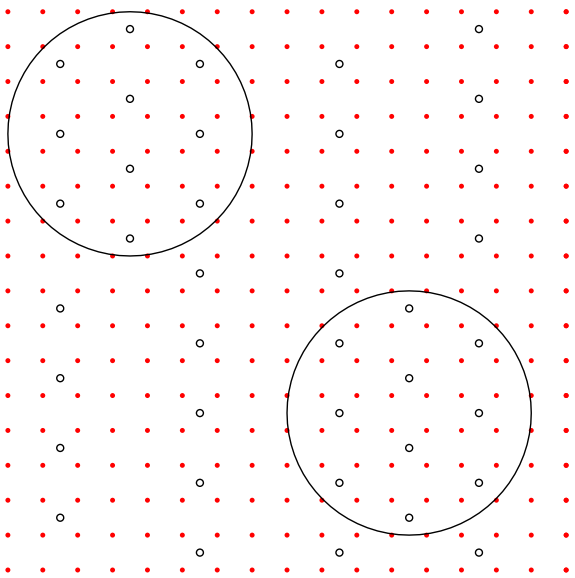

Fig. 1. $CuO_2$ plane and arrangement of dopants (vacancies) in the alkaline earth ion layer for inhomogeneous 14% doping

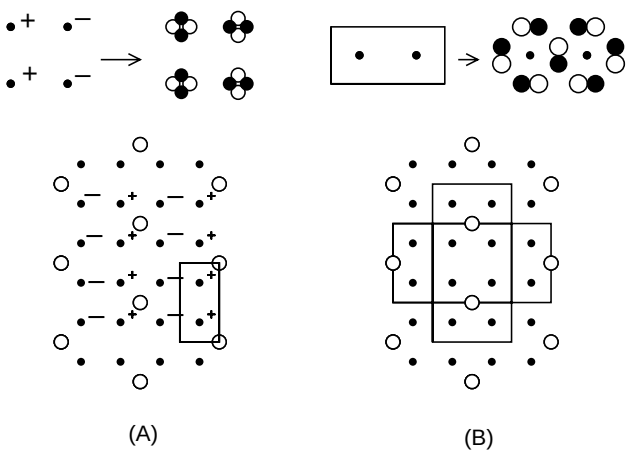


Fig. 2. $\alpha$-spin (A) and $\beta$-spin HOMO (B) of $Cu_{24}O_{50}Ca_6Sr_{15}$


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## References


[1] K.M. Lang, V. Madhavan, J.E. Hoffman, E.W. Hudson, H. Eisaki, S. Uchida ,J.C. Davis: Nature **415** (2002) 412.

[2] J. Tanaka: Int. J. Mod. Phys. B **14** (2000) 3691.

[3] M. Azuma, Z. Hiroi, M. Takano, Y. Bando, Y. Takeda: Nature, **356** (1992) 775.