Substantial evidence for new electron pairing mechanism in high temperature superconductors

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We propose that *the change of the electron clouds* of the transition metal ions (or/and other ions) is the electron pairing medium in high temperature superconductors. It is just like the vibration of the crystal lattice is the electron pairing medium in conventional superconductors. The pairing mechanism is as follows. When a free electron arrives at a new place in the crystal, the electron clouds of the neighboring transition metal ions will change. In this way, the negative charge densities around the free electron will decrease. When the free electron departs, the electron clouds of the transition metal ions will not relax immediately, so that there will form a region lack of negative charge. This is equivalent to the appearance of a positive charge. Another free electron with negative charge will be attracted. Then an attraction between two free electrons appears. This mechanism is essentially the same as the electron-lattice interaction, except that the medium is *the change of the electron clouds*, not the displacement of the ions.

In this article, we will provide substantial evidence.

Table 1 shows the superconducting transition temperatures of three copper oxide superconductors and the frequencies of *the change of the electron clouds* calculated by TDDFT method. The detailed calculation method is described in [1][2][3]. For comparison, Table 2 gives the maximum phonon frequencies and the superconducting transition temperatures of three typical conventional superconductors.

Table 1 Superconducting transition temperatures of three copper oxide superconductors and the frequencies calculated by TDDFT method. $La_{2-x}Sr_xCuO_4$ gives the transition temperature of $La_{2-x}Sr_xCuO_4$ with $x = 0.15$. We found different modes with different frequencies in $La_{2-x}Sr_xCuO_4$ and $TlBa_2CaCu_2O_7$, respectively.

	$La_{2-x}Sr_xCuO_4$	$TlBa_2CaCu_2O_7$	$HgBa_2Ca_2Cu_3O_8$
T_c/K	38	91	133
ω/meV	36, 83 [1]	140, 208 [2]	250 [3]

Table 2 Maximum phonon frequencies and superconducting transition temperature of three typical conventional superconductors.

	Pb	MgB_2	H_3S
T_c / K	7	39	164
ω / meV	9 [4]	90 [4]	250 [5]

First, the calculated frequency of *the change of the electron clouds* is close to that of the crystal lattice. So, the change of the electron clouds can be excited by free electrons. The results are unexpected and disruptive, because the change of the electron density should be very quick according to the Born Oppenheimer Approximation. Our results indicate that the Born Oppenheimer Approximation is not applicable for *the change of the electron clouds.*

Second, for the three copper oxide superconductors $La_{2-x}Sr_xCuO_4$, $TlBa_2CaCu_2O_7$, and $HgBa_2Ca_2Cu_3O_8$, the higher the superconducting transition temperature, the higher the calculated frequency of *the change of the electron clouds.* They exhibit a high degree of correlation.

The results demonstrate that *the change of the electron cloud* is the electron pairing medium in unconventional high temperature superconductors.

The following is images of *the change of the electron clouds* of La_2CuO_4, $TlBa_2CaCu_2O_7$, and $HgBa_2Ca_2Cu_3O_8$.

Fig. 1 shows the crystal structure and the real-time evolution of the charge density of La2CuO4. The change of the electron clouds of Cu^{2+} ions become obvious gradually with the evolution steps. For Cu1, the change of the charge density reaches its maximum after about 1500 steps, and the corresponding time is 3.0 $\hbar$/eV. It is the time from zero to the maximum. The time of one period should be 4×3.0 $\hbar$/eV and the frequency is about 83 meV. For Cu2, the change of the charge density reaches its maximum after about 3500 steps, and the corresponding frequency is about 36 meV.

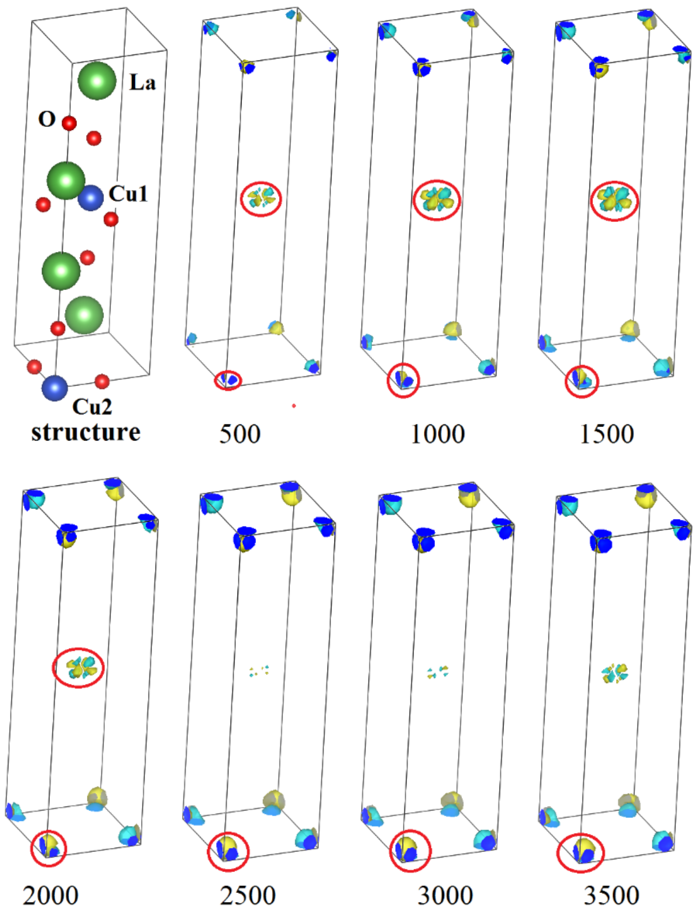

Fig.1 Crystal structure and the change of the electron cloud over time of La_2CuO_4. Plots were generated using VESTA [6]. The iso-surface is 0.05 e/bohr^3.

Fig. 2 shows the results of $TlBa_2CaCu_2O_7$. The change of the electron cloud of the Cu^{2+} ion indicated by an arrow reaches its maximum after about 600 steps. The frequency is approximately 208 meV.

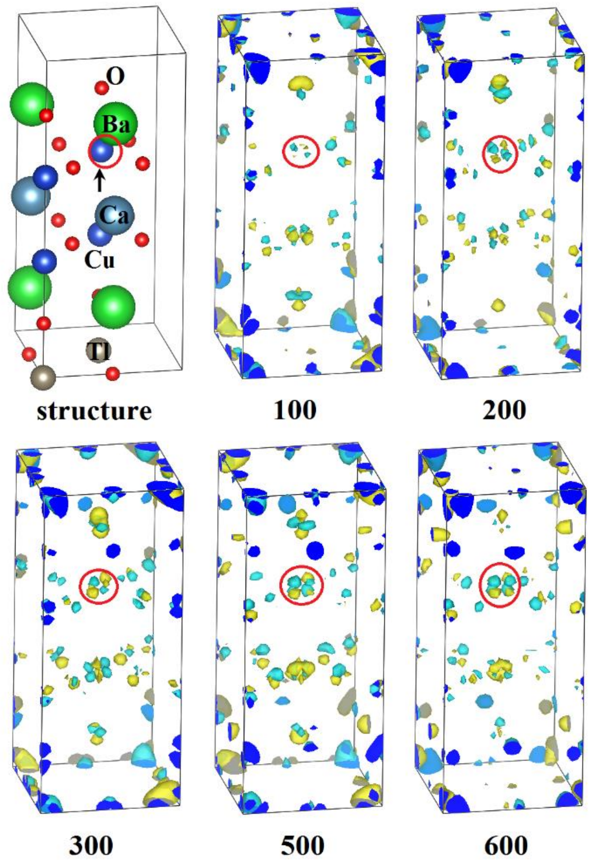

Fig. 2 Crystal structure and the change of the electron cloud over time of $TlBa_2CaCu_2O_7$. The iso-surface is 0.05.

Fig. 3 shows the results of $HgBa_2Ca_2Cu_3O_8$. The change of the electron cloud of the Cu^{2+} ion indicated by the arrow reaches its maximum after about 500 steps. The frequency is approximately 250 meV.

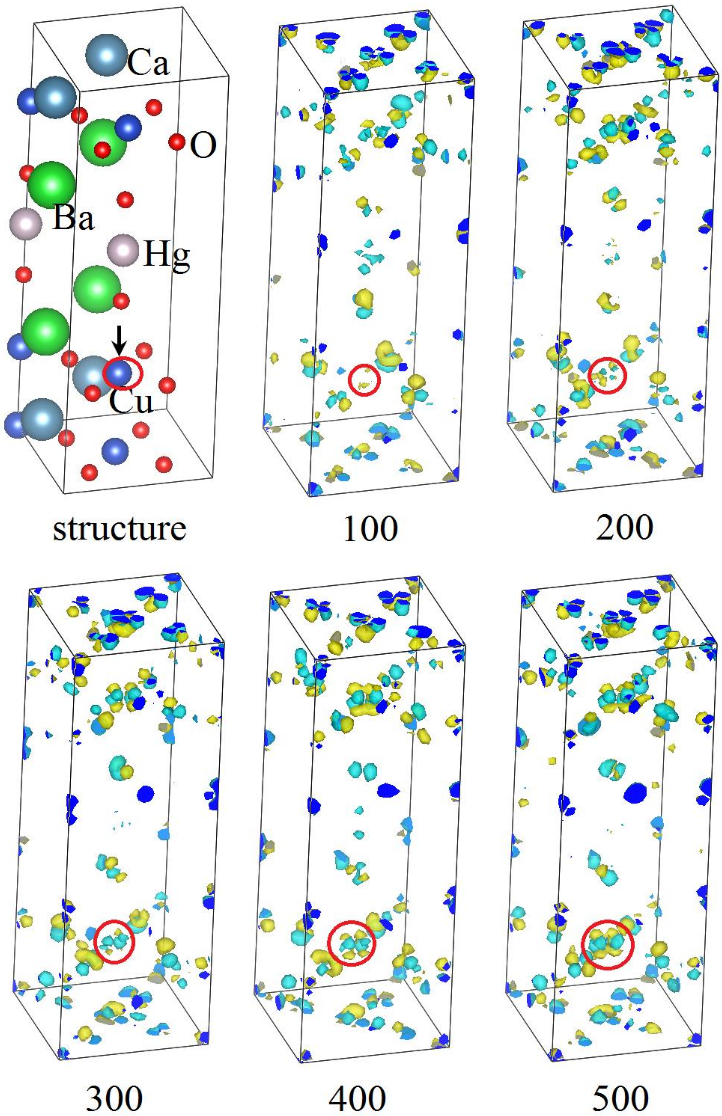

Fig. 3 Crystal structure and the change of the electron cloud over time of $HgBa_2Ca_2Cu_3O_8$. The iso-surface is 0.05.

Reference

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