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Identifying the genes of unconventional high temperature superconductors

Jiangping Hu

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Abstract We elucidate a recently emergent framework in unifying the two families of high temperature (high T_c) superconductors, cuprates and iron-based superconductors. The unification suggests that the latter is simply the counterpart of the former to realize robust extended s-wave pairing symmetries in a square lattice. The unification identifies that the key ingredients (gene) of high T_c superconductors is a quasi two dimensional electronic environment in which the *d*-orbitals of cations that participate in strong in-plane couplings to the *p*-orbitals of anions are isolated near Fermi energy. With this gene, the superexchange magnetic interactions mediated by anions could maximize their contributions to superconductivity. Creating the gene requires special arrangements between local electronic structures and crystal lattice structures. The speciality explains why high T_c superconductors are so rare. An explicit prediction is made to realize high T_c superconductivity in Co/Ni-based materials with a quasi two dimensional hexagonal lattice structure formed by trigonal bipyramidal complexes.

Keywords Cuprates · Iron-based superconductors · Unconventional high T_c superconducotors · Superexchange

J. Hu (✉)
Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
e-mail: jphu@iphy.ac.cn

J. Hu
Collaborative Innovation Center of Quantum Matter, Beijing 100190, China

1 Introduction

Almost three decades ago, the first family of unconventional high T_c superconductors, cuprates [1], was discovered. The discovery triggered intensive research and has fundamentally altered the course of modern condensed matter physics in many different ways. However, even today, after tens of thousands of papers devoted to the materials have been published, understanding their superconducting mechanism remains a major open challenge. Researchers in this field are sharply divided and disagree with each other on many issues arranging from minimum starting models to basic physical properties that are relevant to the cause of superconductivity. There is even a growing skepticism whether there are right questions that can be asked to settle the debate on the superconducting mechanism.

Many reasons can be attributed to the failure of answering the question of how superconductivity arises in cuprates. For example, material complexity makes theoretical modeling difficult, rich physical phenomena blind us from distinguishing main causes from side ones, and insufficient theoretical methods leave theoretical calculation doubtable. However, beyond all these difficulties and the absence of consensus, the lack of successfully realistic guiding principles to search for new high T_c superconductors from theoretical studies is the major reason. The failure was witnessed in the surprising discovery of the second family of high T_c superconductors, iron-based superconductors [2], in 2008. Today, those who are theory builders and those who are material synthesizers still remain disentangled.

Can valuable leads be provided from the theoretical side ahead of the potential discovery of the third family of high T_c superconductors? It is conceivable that the hope to settle high T_c mechanism relies on a positive answer to this question. Here, we believe that it is the time to seek a positive answer based on the following two reasons. First, in the past 7 years, the intensive research on iron-based superconductors has brought much new information. For those who believe that cuprates and iron-based superconductors should share a common high T_c mechanism, an opportunity to settle the debate arises as it is the first time that the traditional inductive reasoning becomes available in research. On one side, iron-based superconductors and cuprates share many common features, but on the other side they are not clones of each other. The similarities and differences can thus speak promising clues. Second, from the past massive searching efforts, it has become increasingly clear that unconventional high T_c superconductors are rare materials. Moreover, for the two known families, their superconductivities are carried robustly on CuO_2 layers in cupates and on FeAs/Se layers in iron-based superconductors respectively. The simultaneous existence of the rareness and robustness suggests that the unconventional high T_c superconductivity is tied to special ingredients in the electronic world, which define the gene of unconventional high T_c superconductivity. Thus, using inductive reasoning to identify the gene can open a new window to search for high T_c superconductors.

In this article, by taking the assumption that a common superconducting mechanism is shared by both known high T_c superconductors, we elucidate a recently emergent path to end the deadlock in solving high T_c mechanism by implementing inductive reasoning to reexamine the high T_c problem [3, 4]. This path stems from a simple framework that unifies cuprates and iron-based superconductors based on previous understandings in repulsive interaction or magnetically driven high T_c mechanisms. It suggests that iron-based superconductors are simply the counterpart of cuprates to realize robust extended s-wave pairing symmetries in a square lattice. Both materials share a key ingredient, the gene of unconventional high T_c superconductivity: a quasi two dimensional electronic environment in which the *d*-orbitals of cation atoms that participate in strong in-plane couplings to the *p*-orbitals of anion atoms are isolated near Fermi energy. This environment allows the antiferromagnetic (AFM) superexchange couplings mediated through anions, the source of superconducting pairing, to maximize their contributions to superconductivity. Creating such a gene is tied to special arrangements between local electronic structures and crystal lattice structures, which explains why cuprates and iron-based superconductors are special and high T_c superconductors are so rare. The framework can be explicitly tested in future experiments as it leads to an explicit prediction to realize high T_c superconductivity in the Co/Ni-based materials with a quasi two dimensional hexagonal lattice structure formed by trigonal bipyramidal (TBP) complexes [3]. The new materials are predicted to be high T_c superconductors with a $d \pm id$ pairing symmetry. If verified, the prediction will establish powerful guiding principles to search for high T_c superconductor candidates, as well as to settle the debate on unconventional high T_c superconducting mechanism.

2 Questions for unconventional high T_c superconductivity

Implementing inductive reasoning to understand both cuprates and iron-based superconductors, we lay out the high T_c problem with the following three subsequent questions:

(1) What is the common interaction responsible for high T_c superconductivity in both families?
(2) What are the key ingredients to make both families special to host high T_c superconductivity?
(3) Where and how can we search for new high T_c superconductors?

The three questions are highly correlated. They form a self-contained unit to reveal high T_c superconducting mechanism.

In the past, the first question was the central question. Its answer was debated wildly. The second question was largely ignored. However, after the discovery of iron-based superconductors, it becomes clearer that the second question should be the central piece. While most researches have concentrated on these two families of high T_c superconductors, it is equally important to answer why numerous materials, which are similar to cuprates or iron-based superconductors in many different ways, do not exhibit high T_c superconductivity. Therefore, the essential logic here is that whatever our answer to the first question is, the answer must provide an answer to the second question. The answer to the second question can provide promising leads to answer the third question. An explicit theoretical prediction of new high T_c superconductors and its experimental verification can finally justify the answer of the first question to end the debate on high T_c mechanism.

3 The ansatz to the first question

We start with the first question. Our proposed answer to the first question is that only the superexchange AFM interactions mediated through anions are responsible for generating superconductivity in both families of high T_c superconductors. We call this ansatz as the selective magnetic pairing rule [4] in the repulsive interaction or